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Official Opening of the ICONAT-2026

3 Sep 2026 09.30

Fethiye Municipality

Cultural Center

Fethiye-Turkiye

PROGRAM

08.30 The Start of Registration Process

09.30 Official Opening of the ICONAT-2026

Welcome by Conference

Prof. Dr. Murad Omarov, Vice-Chairman Organization Committee
Vice-Rector, NURE, Ukraine.

Prof. Dr. Abidin Kılıç, Chairman of Organization Committee
Eskisehir Technical University, Türkiye

INVITED SPEAKERS

3 Sep 2026

10.00 Prof. Dr. Ekrem Aydiner

“Fundamental Problems of Cosmology and Proposed Solutions”
(Kozmolojinin Temel Problemleri ve Çözüm Önerileri)

11.00 Prof. Dr. Yavuz Akbulut

“Is Science Always Right? How Changing Truths Make Science Stronger”
(Bilim Her Zaman Haklı mı? Değişen Doğrular ve Güçlenen Bilim)

12.00 Lunch Break

13.30 Sam SCIMEMI

“From Low-Earth-Orbit, to the Moon and onto Mars”
(Dünya'nın Alçak Yörüngesinden, Ay'a ve Mars'a)

14.30 Prof. Dr. Maryna Yevdokymenko

“Cybersecurity Education For Industry 5.0: A Human-Centric”
(Endüstri 5.0 için Siber Güvenlik Eğitimi: İnsan Odaklı Bir Yaklaşım)

TABLE OF CONTENTS

Poster Presentation's Program				6
Oral Presentation's Program				8
ABSTRACTS				
No	Name Surname	Title	Country	Page
POSTER PRESENTATIONS				
P01	Derya ARSLAN, Şevval ŞEN	EVALUATION OF PECTIN TYPES FOR TEXTURE DEVELOPMENT AND GELATION PERFORMANCE IN FRUIT-BASED CONFECTIONERY APPLICATIONS	Türkiye	13
P02	Şevval ŞEN, Derya ARSLAN	GLASS TRANSITION, WATER ACTIVITY, AND HYGROSCOPICITY IN DRIED FOOD SYSTEMS: A REVIEW	Türkiye	13
P03	Ebru Bozkurt Abdik	ULTRASOUND-ASSISTED EXTRACTION AND IT'S EFFECTS ON NUTRIENT RETENION AND FOOD SHELF STAILIT	Türkiye	14
P04	Zeynep ASILTÜRK	PRODUCTION OF PROTEIN-RICH PRODUCT FRACTIONS FROM OILY SEEDS AND NUTS by SUPERCRITICAL CO ₂ EXTRACTION: A SUSTAINABLE APPROACH for MULTI- COMPONENT VALORIZATION	Türkiye	14
P05	Dilek KELGÖKMEN GÜLEÇ, Şule METE	DEVELOPMENT OF A HIGH-ANTHOCYANIN ARONIA EXTRACT AND ITS COMPARATIVE EVALUATION WITH ELDERBERRY EXTRACT	Türkiye	15
P06	Gülfem Güneydere, Pınar Anıl Hacıdoğan, Şule Mete	EVALUTION OF MALT EXTRACTS AS AN ALTERNATIVE TO CAMEL	Türkiye	15
P07	Müjde Elif BOZKURT, Evrim Burcu UNCÜ KİRTİŞ	RECOVERY OF POST-PROCESSING FOOD WASTE AS DIETARY FIBER AND THEIR CONVERSION INTO VALUE-ADDED PRODUCTS	Türkiye	16
P08	Samira Hamza Reguig, Sarah Zeghada, Ghena Bentabed-Ababsa, Florence Monjin	USE OF CATALYTIC NANOMATERIALS FOR THE SYNTHESIS OF NITROGEN-CONTAINING HETEROCYCLES VIA 1,3-DIPOLAR CYCLOADDITION	Türkiye	16
P09	Onur Kayabaşı, Rengin Özgür, Barış Uzılday	SCREENING OF HIGH-TEMPERATURE STRESS RESPONSES IN <i>ARABIDOPSIS THALIANA</i> COL-0 MUTANTS PRODUCED BY SPACEFLIGHT-INDUCED MUTAGENESIS	Türkiye	17
P10	Olena KOVALENKO ¹ , Olga YUNAKOVA, Mykola YUNAKOV	OPTICAL PROPERTIES OF K ₂ CuCl ₃ THIN FILMS	Ukraine	17
P11	Yuliya Shamsiyeva, Dmitriy Silayev, Azamat Yermukhanov, Bakhtiyar Yakupov, Savva Timochshuk, Daulet Abdishov, Assel Kiribayeva	ENZYMATIC VALORIZATION OF CEREAL STRAW INTO XYLOOLIGOSACCHARIDES USING RECOMBINANT XYLANASE FROM <i>BACILLUS SONORENSIS</i> (WITHDRAWN)	Kazakhstan	18
P12	Sherazad HAMZA REGUIG	COMPARATIVE EFFECTS OF SUBSTITUTING TWO FATS ONE NATURAL AND ONE INDUSTRIAL ON LIPID PEROXIDATION IN RATS MADE OBESE BY A HIGH-FAT DIET	Algeria	18
P13	Yan O. Singo	COMPUTATIONAL CHARACTERIZATION OF ISOGUVAINE INTERACTIONS	Indonesia	19
P14	Alhama Salem	USING COLOR MEASUREMENT METHODS IN DETERMINING GLUCOSE LEVELS	India	19
P15	Omar LAROUK	THE EVOLUTION OF INFORMATION SERVICES IN PROFESSIONAL SOCIAL NETWORKS	France	19
P16	Omar M. ELZAID	THE IMPACT OF LOCAL ATOMIC POLARIZATION ON MEDICAL MAGNETIC FIELD	Libya	20
P17	Karimova Z. TASHEVNA	THE INVESTIGATION OF THE TEACHING OF PHYSICAL EDUCATION	Uzbekistan	20
P18	Patrick S. CLAIR	CLASSIFICATION OF ANTAGONISTIC EFFECTS OF THE MITOCHONDRIAL MATRIX	USA	20
S	Celil Ikram	SYNTHESIS AND CHARACTERIZATION OF COPPER-DOPED CERAMIC PIGMENTS	Bulgaria	21
P20	Nkiru E Ekechukwu	A NOVEL METHOD FOR SPERM QUANTIFICATION IN THE AFRICAN MALARIA MOSQUITO ANOPHELES GAMBIAE S.L.2	Nigeria	21
P21	Mahrumi Saloni	AMMONIA ADSORPTION CAPACITIES OF NATURAL MATERIALS	India	21
P22	Afamefuna Moon	A METHOD USING ARTIFICIAL INTELLIGENCE TO EXAMINE THE ORDERING MODELS OF SYMMETRICAL STRUCTURES	Nigeria	22
P23	Nacip Kumar	SYNTHESIS OF A NOVEL CATIONIC SALT-CONTAINING SURFACTANT POLYMER COMPLEX USING ARTIFICIAL INTELLIGENCE	India	22
P24	Leo. S. Sian	THE EFFECT OF MAGNETIC FIELD APPLICATION PROCESS ON THE STRUCTURE OF NIOBIUM OXIDE FILMS	China	22
P25	Manuela Uberi	UNDERSTANDING AND INVESTIGATING THE ORIGIN OF COSMIC RAYS	Italy	23
P26	Laura Botez	THE IMPACT OF SIFTS IN THE EARTH'S AXIS ON CLIMATE	Romania	23
P27	Wang Xinyi	INCREASING ENERGY EFFICIENCY IN AGRICULTURE WITH ARTIFICIAL INTELLIGENCE AND SELF-GENERATING ENERGY SYSTEMS	China	23
ORAL PRESENTATIONS				
O1	Tugec PEKDOĞAN ¹	FROM MONITORING TO DECISION-MAKING: RETHINKING INDOOR AIR QUALITY ASSESSMENT IN SCHOOL BUILDING	Türkiye	24
O2	Vural AVCI	A SCENARIO-BASED SIMULATION APPROACH IN MUM-T TRAINING. THE APEX-RAMEF CASE STUDY	Türkiye	24
O3	Igor NEVLIUDOV, Shakhin OMAROV, Svitlana SOTNIK, Nataliia DEMSKA	PREDICTIVE MAINTENANCE OF PRODUCTION EQUIPMENT USING ARTIFICIAL INTELLIGENCE METHODS	Ukraine	25
O4	Yan Hong NG, Muhamad Imam MUHAJIR, Rani MAHARANI, Unang SUPRATMAN, Jalifah LATIP, Murni Nazira SARIAN, Su Datt LAM, Shevin Rizal FERROZ	IMPROVED ALBUMIN BINDING PROPERTIES OF ISOGUVACINE UPON ESTERIFICATION	Malaysia	25
O5	Sei Leo	EXPRESSION OF SOME QUANTITIES IN PHYSICS WITH BI-QUATERNION ALGEBRA	China	26
O6	Hakan DAL, Muhammet Recep OKUR	VIRTUAL PHYSICS COURSE LAB APPLICATIONS (VPCLApps): DESIGN AND IMPLEMENTATION OF INNOVATIVE DIGITAL LEARNING ENVIRONMENTS IN PHYSICS EDUCATION	Türkiye	26
O7	Vusala Xudashirin MURADOVA	A DIALOGUE-BASED DECISION-MAKING SYSTEM FOR SOLVING PLANNING PROBLEMS UNDER UNCERTAINTY	Azerbaijan	26
O8	Valeri Maryan	ANALYSIS OF QUADRUPOLE MOMENT OF ATOMIC NUCLEUS WITH OCTONIONS	Bulgaria	27
O9	Chris Benzerouk	CHARACTERIZATION OF AlGaSb NANOCRYSTALLINE PRODUCED BY MECHANICAL	Algeria	27
O10	Hamza ETTADILI, Caner VURAL	MICROBIAL NANOTECHNOLOGY FOR GREEN SYNTHESIS OF SILVER NANOPARTICLES: SCREENING, CHARACTERIZATION, AND ASSESSMENT OF ANTIFUNGAL ACTIVITY	Türkiye	27
O11	Utku Kaya, Ahmet Onay	A SEMI-SUPERVISED LEARNING APPROACH FOR SEGMENTATION OF RAILWAY TRACKS AND STRUCTURAL HEALTH MONITORING	Türkiye	28

O12	Ahmet Onay, Utku Kaya	DETERMINING THE FINANCIAL BEHAVIOR PROFILES OF CONSTRUCTION INSPECTION STUDENTS USING DECISION TREES AND CLUSTER ANALYSIS	Türkiye	28
O13	Louisa XAVIER	ENERGETIC AND MECHANISTIC INSIGHTS INTO CHEMICAL REACTIONS OF THE DISULFIDE BONDINDIMETHYL DISULFIDE: A THEORETICAL APPROACH	France	28
O14	Ömer ŞENTÜRK, Zeynep BATMAZ	EFFECTS OF DATA SPLITTING STRATEGIES ON RECOMMENDER SYSTEM EVALUATION	Türkiye	29
O15	Abdullah Ensarit	MOS AND WSE MONOLAYERS AS ANODE MATERIALS ELECTRIC FIELD EFFECT	Morocco	29
O16	Volodymyr STOROZHENKO, Sergiy MESHKOV, Oleksandr MIAHKYI, Roman OREL	INCREASING THE EFFICIENCY OF THE THERMOGRAPHIC TECHNIQUES FOR EARLY DIAGNOSTICS OF THE TRANSFORMER CONDITION	Ukraine	29
O17	Nihal Kuş	PHOTOISOMERIZATION AND CONFORMATIONAL ANALYSIS OF MATRIX-ISOLATED PHTHALIC ACID	Türkiye	30
O18	CH. Ganesh kumar, Joji Tammisetty, E. Aadi Satya Goud, R. Uma Sai Durga Devi, V. Sri Manju Bhargavi	DECENTRALIZED IDENTITY VERIFICATION USING BLOCK CHAIN	India	30
O19	Muhammet ARUCU, Ahmet AKKAYA	MACHINE LEARNING PREDICTION OF BAND GAPS IN ABX ₃ PEROVSKITES USING OPEN MATERIALS DATABASES AND COMPOSITION-BASED FEATURES	Türkiye	31
O20	Arif KIVRAK, Hilal DEMİR KIVRAK	SUSTAINABLE AND GREEN ORGANIC CATALYST TECHNOLOGIES FOR NEXT-GENERATION FUEL CELLS	Türkiye	31
O21	Nihal KUŞ	THEORETICAL INVESTIGATION OF THE STRUCTURAL, ELECTRONIC, AND VIBRATIONAL PROPERTIES OF 8-CHLOROTHEOPHYLLINE USING DFT AND TD-DFT METHODS	Türkiye	32
O22	Muhammet ARUCU, Mustafa TAŞCI	TRANSFER MATRIX ANALYSIS OF ONE-DIMENSIONAL PHOTONIC CRYSTALS: DESIGN OF BRAGG REFLECTORS AND DEFECT-MODE OPTICAL FILTERS	Türkiye	32
O23	Fadime MERT BALCI	NANOPOROUS METAL OXIDE THIN FILMS VIA SOFT TEMPLATING	Türkiye	33
O24	Ayşe Hatun POYRAZ, Seda BEYAZ	ECO-FRIENDLY SYNTHESIS AND CHARACTERIZATION OF SILVER-COATED SILICON DIOXIDE NANOCOMPOSITES USING HYPERICUM PERFORATUM L	Türkiye	33
O25	Muhammad Zeeshan-Asad, James C. Reynolds, Sandra E. Dann, Simon A. Kondrat	PROMOTER OR POISON? THE EFFECT OF ZnO STABILITY ON CATALYTIC ACTIVITY IN AMINE- ASSISTED CO ₂ HYDROGENATION TO METHANOL	UK	34
O26	Sude Nur HERDURAN, Filiz ALTAN	DETERMINATION OF THE REGULATORY ROLE OF <i>CATHARANTHUS ROSEUS</i> L. ON GLUCOSE METABOLISM AND ADIPOCYTE FUNCTIONS IN 3T3-L1 ADIPOCYTE CELLS	Türkiye	34
O27	Izfa Riza Hazmi, Muhammad Bukhari Kamal Ariffin	COMMUNITY STRUCTURE AND TEMPORAL DYNAMICS OF VESPID WASPS (HYMENOPTERA: VESPIDAE) IN A MALAYSIAN SECONDARY FOREST	Malaysia	34
O28	Volodymyr STOROZHENKO, Sergiy MESHKOV, Roman OREL, Oleksandr MIAHKYI	APPLICATION OF THERMOGRAPHY TO MONITOR PIPELINES LOCATED IN THE SOIL APPLICATION OF THERMOGRAPHY TO MONITOR PIPELINES LOCATED IN THE SOIL	Ukraine	35
O29	Ali Yener BÜYÜKKÖROĞLU Nilüfer ALTUNKAYA ²	PHYSICS COURSE VIRTUAL LABORATORY APPLICATIONS	Türkiye	35
O30	Abror Kurbanov	THE IMPACT OF DAMS ON CLIMATE CHANGE	Uzbekistan	36
O31	Timur TONGUR	SIMULTANEOUS DETERMINATION OF ELEVEN MULTI-CLASS PESTICIDE RESIDUES IN CHERRIES BY LC-MS/MS: METHOD VALIDATION AND REAL SAMPLE ANALYSIS	Türkiye	36
O32	Pınar UÇAN, Orhan ER	A COMPARATIVE ANALYSIS OF FEATURE ENGINEERING TECHNIQUES FOR MACHINE LEARNING-BASED HEART DISEASE PREDICTION	Türkiye	36
O33	Necdet UÇAN, Oğuz Emrah TURGUT	A COMPARATIVE ANALYSIS OF MACHINE LEARNING ALGORITHMS AND FEATURE ENGINEERING TECHNIQUES FOR ANXIETY LEVEL CLASSIFICATION: AN APPLICATION ON THE GAMINGSTUDY DATASET	Türkiye	37
O34	Yunus DOĞAN, Bülent BOZDOĞAN	CLONING, RECOMBINANT EXPRESSION, AND PURIFICATION OF HUMAN PAD4 IN <i>ESCHERICHIA COLI</i> BL21(DE3)	Türkiye	37
O35	Mehmet KARAKOÇ	LIVING INTELLIGENCE (LI) IS LIVING ON INTELLIGENT SYSTEMS (ISs): CAN LI REALLY BE SOMETHING ALIVE WITH THEM?	Türkiye	38
O36	Amarja Bhosale	PREPARATION OF SILICA COATED ALUMINIUM NANOPARTICLES FOR COLORIMETRIC DETERMINATION OF GLUCOSE	India	38
O37	Murad Omarov, Maryna Yevdokymenko	CYBERSECURITY EDUCATION FOR INDUSTRY 5.0: A HUMAN-CENTRIC APPROACH WITHIN THE EU CYBER ECOSYSTEM	Ukraine	39
O38	Baghdad Abdulhameed Abdullah AL-BADANI, Abidin KILIÇ	THE DIRAC EQUATION AS GEOMETRIC NECESSITY: A CLIFFORD-ALGEBRA REFORMULATION	Türkiye	39
O39	N. Tuğbagül ALTAN GÜLGÜN ¹	BENCHMARKING AI MODELS FOR SYMBOLIC TURKISH MAKAM MUSIC GENERATION ON A SYMBOLIC TURKISH MAKAM MUSIC DATASET	Türkiye	39
FULL TEXTS				
F1	EFFECTS OF DATA SPLITTING STRATEGIES ON RECOMMENDER SYSTEM EVALUATION, Ömer ŞENTÜRK, Zeynep BATMAZ			42
F2	MACHINE LEARNING PREDICTION OF BAND GAPS IN ABX ₃ PEROVSKITES USING OPEN MATERIALS DATABASES AND COMPOSITION-BASED FEATURES, Muhammet ARUCU, Ahmet AKKAYA			50
F3	TRANSFER MATRIX ANALYSIS OF ONE-DIMENSIONAL PHOTONIC CRYSTALS: DESIGN OF BRAGG REFLECTORS AND DEFECT-MODE OPTICAL FILTERS, Muhammet ARUCU, Mustafa TAŞCI			56
F4	DETERMINING THE FINANCIAL BEHAVIOR PROFILES OF CONSTRUCTION INSPECTION STUDENTS USING DECISION TREES AND CLUSTER ANALYSIS, Ahmet Onay, Utku Kaya			61
F5	THEORETICAL INVESTIGATION OF THE STRUCTURAL, ELECTRONIC, AND VIBRATIONAL PROPERTIES OF 8-CHLOROTHEOPHYLLINEUSING DFT AND TD-DFT METHODS, Nihal KUŞ			66
F6	PHOTOISOMERIZATION and CONFORMATIONAL ANALYSIS of MATRIX-ISOLATED PHTHALIC ACID, Nihal KUŞ			76

POSTER PRESENTATIONS

15:30-17:00

3 Sep 2026

P-01. Derya Arslan-Türkiye

Evaluation of Pectin Types For Texture Development and Gelation Performance in Fruit-Based Confectionery Applications

P-02. Şevval Şen- Türkiye

Glass Transition, Water Activity, and Hygroscopicity in Dried Food Systems: A Review

P-03. Ebru Bozkurt Abdik-Türkiye

Ultrasound-Assisted Extraction and It's Effects on Nutrient Retention and Food Shelf Stability

P-04. Zeynep Asiltürk- Türkiye

Production of Protein-Rich Product Fractions From Oily Seeds and Nuts By Supercritical Co₂ Extraction: A Sustainable Approach For Multi- Component Valorization

P-05. Dilek Kelgökmen Güleç -Türkiye

Development of A High-Anthocyanin Aronia Extract and Its Comparative Evaluation with Elderberry Extract

P-06. Gülfem Güneydere-Türkiye

Evaluation of Malt Extracts as An Alternative to Caramel

P-07. Müjde Elif Bozkurt- Türkiye

Recovery of Post-Processing Food Waste As Dietary Fiber and Their Conversion Into Value-Added Products

P-08. Samira Hamza Reguig-Algeria

Use of Catalytic Nanomaterials for The Synthesis of Nitrogen-Containing Heterocycles Via 1,3-Dipolar Cycloaddition

P-09. Onur Kayabaşı-Türkiye

Screening of High-Temperature Stress Responses in Arabidopsis Thaliana Col-0 Mutants Produced By Spaceflight-Induced Mutagenesis

P-10. Olena Kovalenko- Ukraine

Optical Properties of K₂CuCl₃ Thin Films

P-11. Assel Kiribayeva-Kazakhstan

Enzymatic Valorization of Cereal Straw into Xylooligosaccharides Using Recombinant Xylanase From Bacillus Sonorensis

P-12. Hamza Reguig Sherazad- Algeria

Comparative Effects of Substituting Two Fats One Natural and One Industrial on Lipid Peroxidation in Rats Made Obese by A High-Fat Diet

P-13. Yan O. Singo -Indonesia

Computational Characterization of The Interactions of Isoguvacine

P-14. Alhama Salem -India

Using Color Measurement Method in Determining Glucose Levels.

P-15. Omar LAROUK-France

Evaluation The Information Services of Professional Social Networks in last ten years.

P-16. Omar M. ELZAID-Libya

Investigation of the effect of local atomic polarization on magnetic fields in the healthcare sector.

P-17. Karimova Z. TASHEVNA-Uzbekistan

The Investigation of The Teaching of Physical Education

P-18. Patrick S. CLAIR-USA

Classification of antagonistic effects of the mitochondrial matrix.

P-19. Celil Ikram-Bulgaria

Synthesis and Characterization of Copper-Doped Ceramic Pigments

P-20. Nkiru E Ekechukwu-Nigeria

A novel method for sperm quantification in the African malaria mosquito Anopheles gambiae s.l.2

P-21. Mahrumi Saloni India

Ammonia Adsorption Capacities of Natural Materials

P-22. Afamefuna Moon-Nigeria

A method using artificial intelligence to examine the ordering models of symmetrical structures.

P-23. Nacip Kumar India

Synthesis of a Novel Cationic Salt-Containing Surfactant Polymer Complex Using Artificial Intelligence

P-24. Leo. S. Sian-China

The Effect of Magnetic Field Application Process on the Structure of Niobium Oxide Films

P-25. Manuela Uberi-Italy

A Study Titled "Understanding and Investigating the Origin of Cosmic Rays"

P-26. Laura Botez-Romania

The Impact of Shifts in the Earth's Axis on Climate

P-27. Wang Xinyi-China

Increasing Energy Efficiency in Agriculture with Artificial Intelligence and Self-Generating Energy Systems



ORAL PRESENTATIONS**Session 1****4 Sep 2026****Chairing****Prof. Dr. Nihal Kuş- Türkiye****09:30-09:45****O-1. Tuğçe Pekoğan- Türkiye***From Monitoring to Decision-Making: Rethinking Indoor Air Quality Assessment in School Buildings***09:45-10:00****O-2. Vural Avcı-Türkiye***A Scenario-Based Simulation Approach in Mum-T Training. The Apex-Ramef Case Study***10:00-10:15****O-3. Svitlana SOTNIK -Ukraine***Predictive Maintenance of Production Equipment Using Artificial Intelligence Methods***10:15-10:30****O-4. Shevin Feroz-Malaysia***Improved Albumin Binding Properties of Isoguvacine Upon Esterification***10:30-10:45****O-5. Sei Leo-China***Expression of Some Quantities in Physics with Bi-quaternion Algebra***Session 2****4 Sep 2026****Chairing****Prof. Dr. Arif Kıvrak- Türkiye****11:00-11:15****O-6. Hakan Dal- Türkiye***Virtual Physics Course Lab Applications (Vpclapps): Design and Implementation of Innovative Digital Learning Environments in Physics Education***11:15-11:30****O-7. Vusala Muradova-Azerbaijan***A Dialogue-Based Decision-Making System for Solving Planning Problems Under Uncertainty***11:30-11:45****O-8. Valeri Maryan-Bulgaria***Analysis of Quadrupole Moment of Atomic Nucleus with Octonions***11:45-12:00****O-9. Chris Benzerouk-Algeria***Characterization of AlGaSb Nanocrystalline Produced by Mechanical***12:00-12:15****O-10. Hamza Ettadılı- Türkiye***Microbial Nanobiotechnology for Green Synthesis of Silver Nanoparticles: Screening, Characterization, and Assessment of Antifungal Activity***BREAK TIME**

Session 3**4 Sep 2026****Chairing****Prof. Dr. Hilal Demir Kıvrak- Türkiye****14:00-14:15****O-11. Utku Kaya -Türkiye***A Semi-Supervised Learning Approach for Segmentation of Railway Tracks and Structural Health Monitoring***14:15-14:30****O-12. Ahmet Onay- Türkiye***Determining The Financial Behavior Profiles of Construction Inspection Students Using Decision Trees and Cluster Analysis***14:30-14:45****O-13. Louisa XAVIER -France***Energetic and Mechanistic Insights into Chemical Reactions of the disulfide bondindimethyl disulfide: A Theoretical Approach***14:45-15:00****O-14. Zeynep Batmaz- Türkiye***Effects of Data Splitting Strategies on Recommender System Evaluation***15:00-15:15****O-15. Abdullah Ensarit-Morocco***MOS And WSE Monolayers as Anode Materials Electric Field Effect***Session 4****4 Sep 2026****Chairing****Dr. Utku Kaya- Türkiye****15:30-15:45****O-16. Oleksandr Miahkyi -Ukraine***Increasing The Efficiency of The Thermographic Techniques For Early Diagnostics of The Transformer Condition***15:45-16:00****O-17. Nihal Kuş- Türkiye***Photoisomerization and Conformational Analysis of Matrix-Isolated Phthalic Acid***16:00-16:15****O-18. Joji Tammisetty-India***Decentralized Identity Verification Using Block Chain***16:15-16:30****O-19. Muhammet Arucu-Türkiye***Machine Learning Prediction of Band Gaps In Abx3 Perovskites Using Open Materials Databases and Composition-Based Features***16:30-16:45****O-20. Arif Kıvrak-Türkiye***Sustainable and Green Organic Catalyst Technologies For Next-Generation Fuel Cells***Session 5****4 Sep 2026****Chairing****Dr. Ahmet Onay-Türkiye****17:00-17:15****O-21. Nihal Kuş- Türkiye***Theoretical Investigation of The Structural, Electronic, and Vibrational Properties of 8-Chlorotheophylline Using Dft and Td-Dft Methods***17:15-17:30****O-22. Muhammet Arucu-Türkiye***Transfer Matrix Analysis Of One-Dimensional Photonic Crystals: Design Of Bragg Reflectors And Defect-Mode Optical Filters***17:30-17:45****O-23. Fadime Mert Balcı-Türkiye***Nanoporous Metal Oxide Thin Films Via Soft Templating***17:45-18:00****O-24. Ayşe Hatun Poyraz-Türkiye***Eco-Friendly Synthesis and Characterization of Silver-Coated Silicon Dioxide Nanocomposites Using Hypericum Perforatum L.***18:00-18:15****O-25. Muhammad Zeeshan Asad-UK***Promoter or Poison? The Effect of ZnO Stability on Catalytic Activity in Amine- Assisted CO₂ Hydrogenation to Methanol*

Session 6**5 Sep 2026****Chairing****Prof. Dr. Hakan Dal-Türkiye****09:30-09:45****O-26. Sude Nur Herduran -Türkiye***Determination of the regulatory role of Catharanthus roseus L. on glucose metabolism and adipocyte functions in 3T3-L1 adipocyte cells***09:45-10:00****O-27. Izfa Riza Hazmi-Türkiye***Community Structure and Temporal Dynamics of Vespidae Wasps (Hymenoptera: Vespidae) In A Malaysian Secondary Forest***10:00-10:15****O-28. Roman Orel-Ukraine***Application of Thermography to Monitor Pipelines Located in The Soil***10:15-10:30****O-29. Ali Yener Büyükköroğlu- Türkiye***Physics Class Virtual Laboratory Applications***10:30-10:45****O-30. Abror Kurbanov- Uzbekistan***The Impact of Dams on Climate Change***Session 7****5 Sep 2026****Chairing****Dr. Nur Uluhan-Türkiye****11:00-11:15****O-31. Timur Tongur -Türkiye***Simultaneous Determination of Eleven Multi-Class Pesticide Residues in Cherries By Lc–Ms/Ms: Method Validation and Real Sample Analysis***11:15-11:30****O-32. Pınar Uçan-Türkiye***A Comparative Evaluation of Individual and Hybrid Feature Engineering Techniques for Machine Learning-Based Heart Disease Prediction***11:30-11:45****O-33. Necdet Uçan-Türkiye***A Comparative Analysis of Machine Learning Algorithms and Feature Engineering Techniques for Anxiety Level Classification: An Application on The Gamingstudy Dataset***11:45-12:00****O-34. Yunus Doğan- Türkiye***Cloning, Recombinant Expression, and Purification of Human Pad4 in Escherichia Coli BL21(De3)***12:00-12:15****O-35. Mehmet. Karakoç- Türkiye***Living Intelligence (Li) Is Living On Intelligent Systems (Iss): Can Li Really Be Something Alive With Them?***BREAK TIME****Session 8****5 Sep 2026****Chairing****Prof. Dr. Hakan Dal-Türkiye****14:00-14:15****O-36. Amarja Bhosale -India***Preparation of Silica Coated Aluminium Nanoparticles for Colorimetric Determination of Glucose***14:15-14:30****O-37. Murad Omarov- Ukraine***Application of The Fuzzy Sets Theory in The Management of Technological Processes for The Production of Automation Technical Means***14:30-14:45****O-38. Maryna Yevdokymenko- Ukraine***Cybersecurity Education For Industry 5.0: A Human-Centric***14:45-15:00****O-39. Baghdad Abdulhameed Abdullah AL-BADANI-Yemen***The Dirac Equation As Geometric Necessity: A Clifford-Algebra Reformulation*

15:00-15:15

O-40. Nigâr Tuğbagül Altan Gülgün-Türkiye

Benchmarking AI Models For Symbolic Turkish Makam Music Generation on A Symbolic Turkish Makam Music Dataset



ABSTRACTS



P01**EVALUATION OF PECTIN TYPES FOR TEXTURE DEVELOPMENT AND GELATION PERFORMANCE IN FRUIT-BASED CONFECTIONERY APPLICATIONS****Derya ARSLAN^{1*}****Şevval ŞEN²**¹ R&D Developer, Döhler Gıda Sanayi A.Ş., Balıkesir, Türkiye² R&D Teamlead, Döhler Gıda Sanayi A.Ş., Balıkesir, Türkiye**ABSTRACT**

Pectin is one of the most widely used hydrocolloids in fruit-based confectionery products due to its ability to provide desirable texture, gel strength, stability, and mouthfeel. However, the functional performance of pectin is highly dependent on its degree of esterification, processing conditions, pH, soluble solids, and the presence of divalent ions. Therefore, the selection of an appropriate pectin type is critical for achieving the desired product structure and processing performance at industrial scale. In this study, different commercial types of pectin were evaluated for their suitability in fruit-based confectionery applications. The pectins were assessed with particular emphasis on their dissolution behavior, ease of incorporation into the formulation, gelation performance, and the resulting product texture. Pectin samples with different functional characteristics were incorporated into model fruit-based systems under controlled processing conditions. The effects of sugar concentration, acidity, hydration conditions, and pectin type on the final structure were comparatively evaluated. The results demonstrated that pectin type had a significant influence on both processing behavior and final product texture. Among the evaluated samples, one of the pectin types showed favorable dissolution characteristics and provided a suitable gel structure and texture for fruit-based confectionery applications. Differences observed between the pectin samples highlighted the importance of optimizing pectin selection together with formulation and process parameters rather than evaluating pectin solely based on its nominal dosage. These findings provide practical insights into the selection and application of pectin in industrial fruit-based confectionery formulations and demonstrate the importance of controlling hydration, pH, sugar concentration, and processing conditions to achieve consistent texture and product quality.

Keywords: Pectin, fruit-based confectionery, texture, hydrocolloids, formulation optimization, industrial applications**P02****GLASS TRANSITION, WATER ACTIVITY, AND HYGROSCOPICITY IN DRIED FOOD SYSTEMS: A REVIEW****Şevval ŞEN¹, Derya ARSLAN²**¹ R&D Teamlead, Döhler Gıda Sanayi A.Ş., Balıkesir, Turkey² R&D Developer, Döhler Gıda Sanayi A.Ş., Balıkesir, Turkey**ABSTRACT**

The physical stability of dried food products is closely linked to their moisture content, water activity (aw), glass transition temperature (Tg), and hygroscopicity. Changes in these properties during drying and storage can lead to increased molecular mobility, stickiness, caking, texture loss, and this lead to reduced product stability. These effects are critical for food systems with high solids content and hygroscopic character, where small fluctuations in moisture can trigger disproportionate changes in physical state.

This review examines the interrelationship between Tg, aw, and hygroscopicity in dried food matrices and evaluates their combined role in determining product stability. Particular attention is given to the plasticizing effect of water on amorphous food components, whereby increasing moisture content lowers the glass transition temperature and enhances molecular mobility within the matrix. The relationship between moisture sorption behavior and Tg is discussed, with emphasis on the transition from a glassy to a rubbery state and its consequences for structural collapse, stickiness, and caking—phenomena commonly observed in powdered and dried food products.

The practical significance of these parameters for drying process design is also addressed. Drying conditions directly determine the final moisture content and water activity of the product, which in turn govern its Tg and physical state. Maintaining the product in a sufficiently stable glassy state, both during processing and storage, is therefore a key consideration in developing drying strategies for hygroscopic materials. Tools such as state diagrams, sorption isotherm modeling (e.g., GAB model), and glass transition prediction (e.g., Gordon-Taylor equation) are highlighted as valuable approaches for anticipating critical moisture and temperature thresholds during process design.

Overall, the literature indicates that a comprehensive understanding of dried food stability requires the simultaneous consideration of Tg, aw, and hygroscopicity rather than treating these parameters in isolation. A clearer understanding of their interplay can help explain common quality defects such as stickiness and caking and support the development and optimization of drying processes for products with improved physical and structural stability.

This review aims to provide a consolidated framework for researchers and process engineers working on hygroscopic dried food systems, linking theoretical principles of glass transition science with their practical implications for drying, formulation, and storage stability.

Keywords: glass transition temperature, water activity, hygroscopicity, molecular mobility, dried food, stickiness, caking, drying

P03

ULTRASOUND-ASSISTED EXTRACTION AND IT'S EFFECTS ON NUTRIENT RETENION AND FOOD SHELF STAILITY

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ABSTRACT

Ultrasound extraction (UE) is a non-thermal technique that uses high-frequency sound waves (20–100 kHz) to enhance the release of bioactive compounds and improve microbial safety in foods. This study investigated the effects of UE on microbial inactivation, vitamin C retention, antioxidant activity, and shelf-life extension in fresh orange juice. A total of 18 juice samples (n = 6 per treatment group: control, 10 min UE, 15 min UE) were analyzed. Vitamin C levels were measured using 2,6-dichlorophenolindophenol (DCPIP) titration, antioxidant activity was determined via the DPPH radical scavenging assay, and microbial load was assessed in CFU/mL. Results showed that 15 minutes of UE reduced microbial load by approximately 90% compared to the control on day 10, while retaining ~90% of vitamin C (versus 60% retention in thermally treated samples). Antioxidant activity increased by 20% in UE-treated samples. Consequently, UE treatment extended the shelf life of fresh orange juice by 3–5 days. These findings demonstrate that ultrasound extraction is an effective non-thermal method for enhancing both the nutritional quality and microbial safety of minimally processed foods.

Keywords: Ultrasound extraction, Shelf life, Vitamin C, Non-thermal processing,

P04

PRODUCTION OF PROTEIN-RICH PRODUCT FRACTIONS FROM OILY SEEDS AND NUTS by SUPERCRITICAL CO₂ EXTRACTION: A SUSTAINABLE APPROACH for MULTI- COMPONENT VALORIZATION

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ABSTRACT

Oily seeds and nuts are valuable raw materials for the production of functional food ingredients due to their naturally high protein and lipid contents. They also play an important role in daily nutrition thanks to the valuable vitamins, minerals, and other nutrients they contain. However, conventional defatting and protein isolation processes may involve elevated temperatures, organic solvents, and multiple downstream purification steps, potentially limiting process sustainability and affecting the quality of the resulting protein fractions. Supercritical extraction technology offers many advantages compared to traditional methods. The fact that the process can be carried out at low temperatures allows the protein to be obtained without degradation, while also preventing the deterioration of other useful components. This ensures high quality in the final product.

This project aimed to obtain protein-rich pulps from different oilseeds and nuts using supercritical extraction technology, a green technology. The project involved studies using sunflower seeds, apricot kernels, pumpkin seeds, and hazelnut raw materials. The obtained products were evaluated in terms of nutritional content and their yields were examined.

Keywords: Oily Seeds, Supercritical CO₂ Extraction, Protein, Defatting

P05

DEVELOPMENT OF A HIGH-ANTHOCYANIN ARONIA EXTRACT AND ITS COMPARATIVE EVALUATION WITH ELDERBERRY EXTRACT

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ABSTRACT

Aronia (*Aronia melanocarpa*) is a rich source of anthocyanins and other bioactive compounds, making it a promising natural source for the development of anthocyanin-rich functional ingredients. In this study, an extraction process was developed and optimized to obtain a high-anthocyanin Aronia extract from the fruit matrix. Different processing parameters were evaluated to maximize anthocyanin recovery and obtain a standardized extract with a high anthocyanin content. The anthocyanin content of the resulting Aronia extract was determined using the pH differential method, and its anthocyanin profile and stability were further evaluated to characterize its functional potential. The optimized process resulted in an Aronia extract containing approximately 11% total anthocyanins, demonstrating the potential of Aronia as a concentrated source of anthocyanins. The obtained Aronia extract was subsequently compared with a commercially standardized elderberry extract, containing approximately 14% total anthocyanins, in terms of anthocyanin content, profile, and stability. These findings highlight the potential of process optimization for producing standardized, anthocyanin-rich Aronia extracts and provide a comparative perspective on Aronia and elderberry as natural sources of anthocyanins.

Keywords: Aronia melanocarpa, Anthocyanin Extraction, Anthocyanin Profile

P06

EVALUTION OF MALT EXTRACTS AS AN ALTERNATIVE TO CARAMEL

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ABSTRACT

Caramel color (E150D) is one of the most commonly used colorants in the food and beverage industry due to its ability to impart dark brown coloration. Nevertheless, the increasing demand for clean-label products has accelerated the search for natural alternatives that can deliver comparable color performance while offering additional sensory benefits. Malt-derived ingredients have emerged as promising candidates because they contribute not only to color development but also to desirable flavor characteristics, thereby supporting a more natural product image. In this study, conventional malt extract, gluten-free malt extract, and percolation malt extract were evaluated as potential alternatives to E150D caramel color.

The selected malt extracts were compared with respect to their color-forming capacity, sensory attributes, and application potential. Instrumental color analysis was conducted to quantify color intensity, while sensory evaluation focused on appearance, aroma, flavor, and overall acceptability. Furthermore, the influence of malt source and processing method on color development, sensory profile, and product performance was investigated. Particular emphasis was placed on gluten-free malt extract as a clean-label option for products designed for gluten-sensitive consumers, whereas percolation malt extract was assessed for its ability to provide intense color together with distinctive roasted flavor characteristics.

The findings demonstrated that all malt-based ingredients contributed to brown color formation while imparting characteristic caramelized and roasted flavor notes. Variations in color intensity and sensory perception among the three malt extracts highlighted the significant influence of raw material selection and extraction technology on final product properties. Conventional malt extract exhibited a well-balanced color and flavor profile, gluten-free malt extract provided a clean-label alternative suitable for specialized formulations, and percolation malt extract showed superior coloring potential for applications requiring darker shades.

Overall, malt extracts represent promising natural substitutes for E150D caramel color. Their combined functionality as both coloring and flavoring ingredients offers valuable formulation opportunities for clean-label food products while enabling manufacturers to better meet evolving consumer preferences and market demands, while enabling manufacturers to meet evolving consumer expectations.

Keywords: E150D, caramel color alternative, malt extract, gluten-free malt extract, percolation malt extract, clean label, natural coloring, food applications.

P07

RECOVERY OF POST-PROCESSING FOOD WASTE AS DIETARY FIBER AND THEIR CONVERSION INTO VALUE-ADDED PRODUCTS

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ABSTRACT

With the continuous growth of the global population, food production and consumption have increased substantially, resulting in the generation of large quantities of food waste. Food industry by-products are increasingly recognized as valuable resources due to their potential for recovery and reuse. Their reprocessing not only contributes to waste reduction and environmental sustainability but also enables the recovery of valuable components that can be transformed into high-value-added food products. Dietary fiber has gained considerable attention due to its important role in maintaining human health and its contribution to healthy dietary patterns. Many fruit and vegetable processing by-products, including peels, pulp, seeds, and pomace, are naturally rich in dietary fiber and may therefore serve as promising sources for fiber recovery. Examples include apple, strawberry, red beet, black carrot, tea, apricot, tomato, and watermelon processing residues. Dietary fiber can be recovered from these by-products through various processing techniques, including drying, pretreatment, extraction, and purification. These processes can significantly influence the physicochemical and functional properties of the resulting fiber. Particle size, fiber type, processing conditions, and usage level are among the key factors affecting the technological performance and nutritional quality of fiber-enriched products. Therefore, the selection of appropriate processing methods and formulation conditions is essential for obtaining products with desirable properties. In this context, the present study focuses on the valorization of food industry by-products as sources of dietary fiber and investigates their potential applications in different food products. Particular emphasis is placed on the sustainable use of fruit and vegetable pomace by applying necessary processing technologies to transform these by-products into value-added food ingredients with enhanced nutritional and functional properties. This approach highlights the potential of dietary fiber recovery as an effective strategy for supporting sustainable food production and promoting the circular economy in the food industry.

Keywords: Dietary fiber, apple pomace, particle size, sustainability.

P08

USE OF CATALYTIC NANOMATERIALS FOR THE SYNTHESIS OF NITROGEN-CONTAINING HETEROCYCLES VIA 1,3-DIPOLAR CYCLOADDITION

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ABSTRACT

1,2,3-Triazoles constitute an important class of nitrogen-containing heterocycles in the fields of chemistry and medicine; they possess a wide range of medicinal properties, such as anti-inflammatory¹, antitumor² and antifungal activities³. These compounds can be obtained through various reactions and in the presence of various catalysts. The use of nanomaterials has recently emerged as a highly significant sector in the field of catalysis.⁴

This study aims to investigate the catalytic properties of copper-doped titanate nanotubes (Cu/TiNTs) for the synthesis of 1,2,3-triazoles via microwave irradiation. The catalysts were prepared in two steps: hydrothermal synthesis followed by urea-based precipitation. Regarding the synthesis of heterocycles, it was found that these doped nanotubes effectively catalyze the cycloaddition reaction between aryl azides and activated alkenes under both conventional heating and microwave irradiation.

High yields of 1,2,3-triazoles, reaching 99%, were obtained. Finally, the fungicidal activity of some of the synthesized 1,2,3-triazoles was evaluated.⁵

Keywords: 1, 2, 3-triazoles, nanotube, nanomaterials, fungicidal activity.

P09

SCREENING OF HIGH-TEMPERATURE STRESS RESPONSES IN *ARABIDOPSIS THALIANA* COL-0 MUTANTS PRODUCED BY SPACEFLIGHT-INDUCED MUTAGENESIS

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ABSTRACT

Developing heat-tolerant crops has become an urgent goal for food security under climate change. Conventional mutagenesis approaches such as chemical mutagens and gamma irradiation produce a relatively narrow mutation spectrum. The space environment offers a broader source of genomic variation through cosmic radiation, microgravity, and a weak geomagnetic field, which makes it a promising and still largely unexplored route for crop improvement. Working with such large mutant populations, however, requires screening methods that are both scalable and objective. In this study, *Arabidopsis thaliana* (Col-0) seeds were flown aboard the Shijian-19 satellite under the coordination of the Turkish Space Agency (TUA) in cooperation with the Asia-Pacific Space Cooperation Organization (APSCO). The seeds were exposed to microgravity and cosmic radiation for 13.5 days in low Earth orbit. This represents Türkiye's first space mutagenesis experiment. After the seeds returned, they were germinated to establish a mutant library of approximately 900 genotypes. Space-derived lines were then treated with a one-hour heat shock at 50 °C before sowing. This treatment delayed germination onset by one day and reduced the germination rate by about 40 percent compared to controls. Candidate lines were ranked using standardized germination-rate and fresh-weight scores, which identified approximately 40 top-performing genotypes for further evaluation. To screen this population efficiently, we developed a high-throughput phenotyping pipeline based on Python and OpenCV. The pipeline automatically crops individual Petri-dish scans, processes them in batches, and measures traits within a defined region of interest. The same Petri-dish scans can also be used to extract projected plant and leaf-area measurements, extending the range of traits without additional experiments. This work provides a reproducible, image-based screening platform that combines space mutagenesis with high-throughput phenotyping. It offers a practical foundation for the biochemical and molecular characterization of candidate lines and for the selection of heat-resilient genotypes in future work.

Keywords: Space mutagenesis, *Arabidopsis thaliana*, Heat stress, High-throughput phenotyping, Plant breeding

P10

OPTICAL PROPERTIES OF K₂CuCl₃ THIN FILMS

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ABSTRACT

Ternary compounds of potassium and copper halides were chosen as the subjects of study. This choice was motivated by the growing interest in non-toxic copper perovskites, which could become an alternative to toxic lead perovskites used in optoelectronics, light-emitted diodes (LEDs), displays, photodetectors, and other devices.

The KCl – CuCl system produces only one compound with a stable absorption spectrum, K₂CuCl₃, which significantly simplifies the preparation of a single-phase ternary compound. Thin films of the investigated compound were prepared by vacuum evaporation of a melt of pure KCl and CuCl powders of stoichiometric composition onto quartz substrates heated to 100°C, followed by annealing the films for an hour at the same temperature. This method allows the production of single-phase K₂CuCl₃ films without any admixture of the original components.

The absorption spectrum of the K₂CuCl₃ thin film was studied in the spectral range of 2–6 eV, and a temperature range of 90–333 K. Analysis of the spectrum revealed the cationic nature of excitons in the compound. The exciton spectrum of the compound was interpreted based on transitions in the Cu⁺ ion. The influence of exciton-phonon interaction on the absorption spectrum of K₂CuCl₃ was studied. The one-dimensional (1D) nature of excitons was established from the temperature dependence of the broadening $\Gamma(T)$ of the intense long-wavelength exciton band A

Keywords: thin films, absorption spectra, excitons, copper perovskites.

P11

ENZYMATIC VALORIZATION OF CEREAL STRAW INTO XYLOOLIGOSACCHARIDES USING RECOMBINANT XYLANASE FROM *BACILLUS SONORENSIS*

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ABSTRACT

Agricultural residues such as cereal straw represent abundant renewable resources that can be converted into high-value bioproducts through environmentally friendly biotechnological processes. In this study, wheat (*Triticum aestivum* L.), rice (*Oryza sativa* L.), barley (*Hordeum vulgare* L.), and oat (*Avena sativa* L.) straw were evaluated as feedstocks for the enzymatic production of xylooligosaccharides (XOS) using a recombinant xylanase from *Bacillus sonorensis*.

Enzymatic hydrolysis was carried out under optimized conditions ($200-400 \text{ U g}^{-1}$, 40°C , pH 7.0) using a stepwise enzyme addition strategy (60/40). XOS production depended on both substrate type and enzyme loading. The highest XOS yield was obtained from wheat straw ($40.08 \pm 2.17 \text{ g kg}^{-1}$), followed by barley ($36.87 \pm 0.46 \text{ g kg}^{-1}$), oat ($32.33 \pm 1.18 \text{ g kg}^{-1}$), and rice straw ($27.55 \pm 1.86 \text{ g kg}^{-1}$).

Thin-layer chromatography demonstrated that xylobiose (X2) and xylotriose (X3) were the predominant hydrolysis products. FTIR and ^1H NMR analyses confirmed the carbohydrate nature of the hydrolysates and verified the presence of β -linked xylooligosaccharides. SEM analysis revealed substrate-dependent structural changes after hydrolysis, with more extensive surface disruption observed in wheat and oat straw than in rice and barley.

The results demonstrate the potential of enzymatic processing as a sustainable strategy for the valorization of cereal straw into value-added xylooligosaccharides, which may serve as promising functional ingredients with prospective applications in animal nutrition and other biotechnological sectors.

Keywords: cereal straw; xylanase; xylooligosaccharides; biomass valorization; enzymatic hydrolysis.

P12

COMPARATIVE EFFECTS OF SUBSTITUTING TWO FATS ONE NATURAL AND ONE INDUSTRIAL ON LIPID PEROXIDATION IN RATS MADE OBESE BY A HIGH-FAT DIET

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ABSTRACT

The majority of obesity-related complications are comorbidities such as coronary heart disease, hypertension, type 2 diabetes, respiratory disorders, and dyslipidemia. Margarines contain unsaturated fats, some of which are known for their beneficial effects on cardiovascular risk prevention. However, they can also contain partially hydrogenated fats, which, in large quantities, can lead to cardiovascular complications. The impact of replacing two dietary fats of different origin (industrial or natural) is studied on dyslipidemia and lipid peroxidation of adipose tissue in obese rats. The method is as follows: Obese male rats weighing $400 \pm 10 \text{ g}$ were divided into 2 groups ($n=24$) and consumed 20% margarine or sardine oil for 1 month. On day 30, 6 rats from each group were sacrificed and the remaining rats were then subjected to a diet change for 1 month: margarine was replaced by sardine oil and vice versa. Substituting sardine oil for margarine has no effect on dyslipidemia. In contrast, when margarine is replaced by sardine oil, cholesterol and triglyceridemia are reduced by 35% and 57%, respectively. The levels of thiobarbituric acid-reactive substances and hydroperoxides are lowered by 14% when sardine oil is replaced by margarine and by 18% when margarine is substituted by sardine oil. In contrast, replacing margarine with sardine oil increases hydroperoxide levels (+23%), but these values are lowered (-50%) when sardine oil is substituted by margarine. Replacing margarine with sardine oil reduces high-fat diet-induced hypercholesterolemia and hypertriglyceridemia. In contrast, substituting sardine oil for margarine appears to be more effective against lipid peroxidation.

Keywords: Rats, obesity, dyslipidemia, peroxidation

P13

COMPUTATIONAL CHARACTERIZATION OF ISOGUVACINE INTERACTIONS

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ABSTRACT

Isoguvacine is a highly selective GABA_A receptor agonist widely used in neurochemical research. However, its chemical structure presents a significant challenge: it naturally exists as a zwitterion (a molecule with simultaneous positive and negative charges). Computational studies using Density Functional Theory (DFT) show that this rigid charge layout makes the molecule extremely hydrophilic (water-loving), completely preventing it from crossing the blood-brain barrier (BBB) on its own.

To overcome this limitation, computational modeling plays a key role in designing and testing lipophilic (fat-soluble) prodrug modifications. Molecular Docking simulations demonstrate that while native isoguvacine fits tightly into the receptor pocket via electrostatic salt bridges and hydrogen bonds, adding longer carbon chains (such as ester derivatives) preserves these vital active-site interactions perfectly. Furthermore, Molecular Dynamics (MD) simulations show that these engineered modifications significantly improve the drug's transport behavior. Unlike native isoguvacine, which has negligible affinity for Human Serum Albumin (HSA), the modified versions use their new carbon chains as anchors to slide into the protein's hydrophobic pockets. This allows the drug to be safely carried through the bloodstream and effectively cross the BBB to reach its target receptors in the brain.

Keywords: Isoguvacine, Receptor, Density Functional Theory.

P14

USING COLOR MEASUREMENT METHODS IN DETERMINING GLUCOSE LEVELS

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ABSTRACT

Colorimetric measurement offers a highly simple, cost-effective, and rapid optical method for determining glucose levels across clinical and point-of-care testing applications. The core mechanism relies on specific enzymatic cascades, where glucose oxidase converts glucose into hydrogen peroxide, subsequently triggering a chromogenic agent to change color. Traditionally quantified using desktop spectrophotometers, modern advancements utilize digital color analysis through smartphones, RGB sensors, and computational colorimetric algorithms to detect subtle shifts in hue, saturation, and intensity. By integrating nanomaterials—such as metal nanoparticles that mimic enzyme behaviors—recent systems achieve vastly enhanced analytical sensitivity and lower detection limits. This non-invasive and high-throughput approach bridges the gap between laboratory accuracy and accessible, real-time health monitoring for diabetes management.

Keywords: Colorimetric, glucose levels, RGB sensors.

P15

THE EVOLUTION OF INFORMATION SERVICES IN PROFESSIONAL SOCIAL NETWORKS

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ABSTRACT

Over the past ten years, information services on professional social networks like LinkedIn have changed completely. They used to be simple digital resume folders where people only went to look for a job. Today, they have transformed into active, AI-powered knowledge hubs where professionals go every day to learn, share insights, and track business trends.

The biggest change in these ten years is how information is found and shared. In the past, users had to search for jobs or articles using simple keywords. Today, smart computer programs (algorithms) look at a user's skills, reading habits, and professional network. Then, they automatically suggest the most relevant job openings, industry news, and connections.

Content sharing has also grown immensely. Platforms now offer built-in newsletters, live video streams, and learning courses (like LinkedIn Learning). These tools allow regular workers to create content and become trusted experts in their fields. On the business side, these networks now provide advanced data analytics. Companies use this data to find top talent and target specific business clients. In short, over the last decade, professional networks have shifted from simple contact lists into the most powerful data engines in the modern business world.

Keywords: information services, data analytics.

P16

THE IMPACT OF LOCAL ATOMIC POLARIZATION ON MEDICAL MAGNETIC FIELDS

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ABSTRACT

The interaction between local atomic polarization and magnetic fields serves as a cornerstone for modern medical diagnostics, precision therapeutics, and clinical safety protocols. Atomic polarization—the alignment or deformation of atomic and nuclear spins in response to an external field—directly dictates the efficacy and resolution of advanced healthcare technologies.

In medical imaging, this phenomenon is best demonstrated by Magnetic Resonance Imaging (MRI). High-strength static magnetic fields polarize hydrogen nuclei within human tissue, aligning their spins to create a measurable net magnetization. When perturbed by radiofrequency pulses, the unique relaxation pathways of these polarized atoms allow for high-contrast, non-invasive imaging of soft tissues and organs. Furthermore, advanced hyperpolarization techniques—which use lasers to artificially boost the spin alignment of noble gases like Xenon-129—have revolutionized pulmonary medicine by enabling real-time, high-resolution visualization of lung ventilation and gas exchange.

Beyond structural diagnostics, controlling atomic polarization is critical for ultra-sensitive quantum sensing. Spin-Exchange Relaxation-Free (SERF) magnetometers utilize intensely polarized alkali metal vapors to detect the incredibly faint magnetic fields generated by human brain activity. This application, known as Magnetoencephalography (MEG), allows clinicians to map neurological functions and pinpoint epileptic focuses without surgical intervention. In therapeutics, the dynamic manipulation of polarization fields drives targeted oncology treatments. By applying alternating magnetic fields to localized iron-oxide nanoparticles inside tumors, rapid polarization reversals generate frictional heat (magnetic hyperthermia) that selectively destroys cancer cells while sparing healthy tissue.

Finally, understanding these microscopic field interactions is vital for occupational health. As clinical facilities transition to ultra-high-field systems (7 Tesla and above), rapid movement through strong magnetic gradients can induce transient electrical polarization changes in human tissue. This frequently causes benign, temporary physiological effects among healthcare workers, such as vertigo, nausea, and magnetophosphenes (visual flashes). Consequently, mapping local atomic and molecular responses remains essential not only for pioneering next-generation medical devices but also for establishing rigorous international safety guidelines for clinical environments.

Keywords: magnetometers, atomic polarization, Magnetoencephalography.

P17

THE INVESTIGATION OF THE TEACHING OF PHYSICAL EDUCATION

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ABSTRACT

The investigation of teaching physical education (PE) focuses on how teachers deliver lessons, how students react, and the challenges schools face. Recent studies show that modern PE teachers prefer interactive, student-centered learning styles over old-fashioned drills. When teachers use these engaging methods, they feel happier and more satisfied with their jobs. Research also indicates that future PE teachers generally start their careers with highly positive attitudes and a strong sense of duty.

However, the field faces several major challenges. Many PE teachers report that school administrators prioritize academic subjects like math or science, leaving PE with low budgets and poor equipment. This lack of resources and proper training can lower teacher motivation. To fix these issues and make classes more exciting, researchers are looking into digital tools. Adding wearable fitness trackers and active video games helps track student health accurately and keeps children motivated to stay active.

Keywords: physical education, engaging methods.

P18

CLASSIFICATION OF ANTAGONISTIC EFFECTS OF THE MITOCHONDRIAL MATRIX

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ABSTRACT

The mitochondrial matrix is the central hub for cellular energy production, metabolism, and quality control. Antagonistic effects within this compartment refer to the opposing forces, signals, or pathways that balance cell survival against cell death. These effects can be classified into three primary areas: protease compartmentalization, metal ion interactions, and reactive oxygen species (ROS) signaling.

First, mitochondrial proteases exhibit a striking spatial antagonism. While matrix proteases (like Lon1) are essential for removing damaged proteins and maintaining lifespan, proteases in the intermembrane space (like Yme1) can sometimes limit mitochondrial respiration. Second, metal toxicity involves antagonistic competition. Heavy metals like cadmium damage matrix enzymes, but essential metals like zinc can block these toxic sites, acting as a natural shield. Finally, ROS signaling creates a metabolic tug-of-war. Low levels of matrix oxidative stress trigger adaptive survival responses, whereas high levels trigger inflammation and programmed cell death. Understanding these antagonistic mechanisms is crucial, as their imbalance directly leads to cellular aging, metabolic diseases, and neurodegenerative disorders.

Keywords: mitochondrial matrix, antagonistic effects, mitochondrial proteases.

P19

SYNTHESIS AND CHARACTERIZATION OF COPPER-DOPED CERAMIC PIGMENTS

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ABSTRACT

Copper-doped ceramic pigments are advanced inorganic colorants synthesized by incorporating copper ions (Cu^{2+}) into crystalline host matrices—such as spinels, apatites, or simple oxides. Produced primarily through high-temperature solid-state sintering, sol-gel synthesis, or coprecipitation methods, these pigments achieve color through $d-d$ electronic transitions of the copper chromophore, resulting in vibrant blue, green, turquoise, and black shades. Modern research characterizes their properties using XRD for phase purity, SEM/TEM for nanoparticle morphology, and UV-Vis spectroscopy for optical bandgap evaluation. Beyond traditional ceramic decoration, copper doping optimizes the pigments for functional applications, including photocatalysis and high solar-reflectance coatings.

P20

A NOVEL METHOD FOR SPERM QUANTIFICATION IN THE AFRICAN MALARIA MOSQUITO ANOPHELES GAMBIAE S.L.2

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ABSTRACT

A novel, highly accurate method for sperm quantification in *Anopheles gambiae s.l.* relies on quantitative Polymerase Chain Reaction (qPCR). This approach replaces traditional, labor-intensive manual microscope counting, which is highly prone to human error due to severe sperm clumping. DNA Extraction: Total DNA is extracted directly from the male testes or the female sperm-storage organ (the spermatheca) after mating. Target Amplification: The protocol utilizes specific primer sets targeting single-copy genes or specific single-nucleotide polymorphisms (SNPs) characteristic of the *Anopheles gambiae* complex. Quantification via Standard Curves: Because each sperm cell contains a consistent, predictable amount of genomic DNA, researchers can calculate the absolute number of sperm cells by comparing the cycle threshold (C_t) values against a pre-established standard curve.

P21

AMMONIA ADSORPTION CAPACITIES OF NATURAL MATERIALS

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ABSTRACT

Agricultural waste, specifically banana peels, was utilized to synthesize high-performance biochars to capture gas-phase ammonia (NH_3). The raw material underwent pyrolysis at 600 °C, followed by chemical activation using potassium hydroxide (KOH) at temperatures ranging from 600 °C to 900 °C. The structural characteristics of the resulting porous carbons were analyzed, revealing that increasing the activation temperature expanded the specific surface area from 1,134 to 2,332 m^2g^{-1} .

Gas-phase adsorption tests demonstrated that the biochar activated at 600 °C (B-KOH-600) achieved the highest efficiency. It reached a maximum ammonia adsorption capacity of 5.94 mmol/g at 0 °C and 3.83 mmol/g at 20 °C. Crucially, the findings indicate that NH_3 capture performance depends heavily on surface chemistry rather than total surface area. Higher activation temperatures reduced the number of acidic functional groups on the carbon surface. Because ammonia is alkaline, it binds primarily to these surface acidic groups via chemical interactions. Consequently, the biochar with the highest concentration of acidic groups (2.30 mmol/g) exhibited the top performance. This study confirms that banana peel waste can be converted into a low-cost, sustainable, and highly efficient green adsorbent for industrial air filtration and ammonia emission control.

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Keywords: Agricultural waste, banana peels, biochar.

P22

A METHOD USING ARTIFICIAL INTELLIGENCE TO EXAMINE THE ORDERING MODELS OF SYMMETRICAL STRUCTURES

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ABSTRACT

Symmetrical structures form the backbone of advanced material design, crystallographic research, and structural engineering. However, modeling and optimizing their underlying ordering patterns traditionally require intensive computational resources and rigid manual constraints. This paper presents a novel framework utilizing equivariant and invariant artificial intelligence architectures to automatically detect, analyze, and optimize ordering models within symmetrical configurations. By embedding geometric and group-theoretic constraints directly into neural network architectures, our approach eliminates the need for exhaustive data augmentation and accurately maps complex physical structures into low-dimensional latent spaces. We demonstrate the efficacy of our method across diverse applications, including crystal lattice optimization and mechanical metamaterial design. The results show that our AI-driven framework significantly reduces computational overhead while maintaining high structural fidelity. Ultimately, this approach establishes a scalable, generalized pathway for the automated discovery and formal verification of highly ordered symmetrical systems. Symmetrical structures form the backbone of advanced material design, crystallographic research, and structural engineering. However, modeling and optimizing their underlying ordering patterns traditionally require intensive computational resources and rigid manual constraints. This paper presents a novel framework utilizing equivariant and invariant artificial intelligence architectures to automatically detect, analyze, and optimize ordering models within symmetrical configurations. By embedding geometric and group-theoretic constraints directly into neural network architectures, our approach eliminates the need for exhaustive data augmentation and accurately maps complex physical structures into low-dimensional latent spaces. We demonstrate the efficacy of our method across diverse applications, including crystal lattice optimization and mechanical metamaterial design. The results show that our AI-driven framework significantly reduces computational overhead while maintaining high structural fidelity. Ultimately, this approach establishes a scalable, generalized pathway for the automated discovery and formal verification of highly ordered symmetrical systems.

Keywords: Symmetrical structures, advanced material design, crystallographic research.

P23

SYNTHESIS OF A NOVEL CATIONIC SALT-CONTAINING SURFACTANT POLYMER COMPLEX USING ARTIFICIAL INTELLIGENCE

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ABSTRACT

Cationic surfactant-polymer complexes play a pivotal role in the development of antimicrobial coatings, smart drug delivery vectors, and advanced functional materials. However, discovering and optimizing these intricate supramolecular networks via traditional empirical chemistry is severely bottlenecked by vast chemical design spaces and highly non-linear electrostatic phase behaviors. This study introduces an artificial intelligence (AI)-driven framework to accelerate the inverse design, optimization, and synthesis of a novel cationic salt-containing surfactant-polymer complex. A Generative Adversarial Network (GAN) was trained on historical chemical datasets to predict and propose unique molecular configurations satisfying predefined performance metrics, including targeted critical micelle concentration (CMC), surface tension reduction, and thermal stability. The self-assembly dynamics of the AI-generated candidates were structurally validated through molecular dynamics (MD) simulations, while reaction parameters—such as molar ratios, pH, and temperature—were systematically mapped using a Bayesian optimization algorithm. Utilizing a closed-loop automated laboratory workflow, the optimized complex was successfully synthesized with high chemical yield. Post-synthesis characterization via FTIR, NMR, and Zeta potential analysis confirmed that the physical complex closely matched the AI's structural predictions with a fidelity exceeding 94%. These findings demonstrate that integrating machine learning into macromolecular synthesis effectively bypasses conventional R&D bottlenecks, establishing a robust paradigm for the rapid discovery of next-generation smart materials.

Keywords: Artificial Intelligence, Cationic Surfactant, Polymer Complex, Inverse Design, Bayesian Optimization, Macromolecular Synthesis.

P24

THE EFFECT OF MAGNETIC FIELD APPLICATION PROCESS ON THE STRUCTURE OF NIOBIUM OXIDE FILMS

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ABSTRACT

In this study, the effect of magnetic field application during the deposition process on the structural and morphological properties of niobium oxide (Nb_2O_5) thin films was systematically investigated. The films were synthesized on silicon (100) and fused silica substrates using reactive magnetron sputtering under varying magnetic field intensities (ranging from 0 mT to 150 mT) and spatial configurations. The crystal structure, surface topography, and chemical composition of the deposited films were characterized using X-ray diffraction (XRD), Atomic Force Microscopy (AFM), Field Emission Scanning Electron Microscopy (FE-SEM), and X-ray Photoelectron Spectroscopy (XPS).

The results demonstrate that the application of an external magnetic field significantly enhances plasma confinement and modulates the kinetic energy of the arriving ionic species. XRD analysis revealed a distinct structural transition from an amorphous matrix to highly oriented crystalline phases (Nb_2O_5) as the magnetic field intensity increased, accompanied by a reduction in lattice strain. AFM and FE-SEM micrographs indicated that optimized magnetic field configurations suppress column boundaries, leading to ultra-smooth surface topographies, a denser microstructure, and a substantial reduction in pinhole defects. Furthermore, XPS data confirmed that the enhanced plasma activation under stronger magnetic fields promotes complete oxidation, resulting in high stoichiometric uniformity across the film depth. These findings suggest that tailoring the magnetic field application process provides a precise, non-thermal pathway to engineer the structural properties of niobium oxide films for high-performance optoelectronic and electrochromic devices.

Keywords: Niobium oxide, Thin films, Magnetic field, Plasma confinement, Microstructure, Magnetron sputtering.

P25**UNDERSTANDING AND INVESTIGATING THE ORIGIN OF COSMIC RAYS****Manuela Uberi**

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ABSTRACT

Cosmic rays—high-energy charged particles traveling through space at nearly the speed of light—have perplexed and fascinated astrophysicists since their discovery over a century ago. Despite their ubiquity, identifying the exact sources of these particles remains one of the greatest challenges in modern astrophysics due to magnetic fields deflecting their trajectories. This paper provides a comprehensive overview of the current understanding of cosmic ray origins, distinguishing between galactic cosmic rays accelerated by supernova remnants and ultra-high-energy extragalactic cosmic rays originating from active galactic nuclei (AGN). Furthermore, we examine the multi-messenger approaches used to investigate these particles, highlighting the critical roles of gamma-ray astronomy, neutrino detection, and ground-based air shower arrays. By synthesizing recent observational data and theoretical acceleration models, this study underscores how tracking these cosmic messengers enhances our understanding of the high-energy processes shaping the universe.

Keywords: Cosmic Rays, Astrophysics, Supernova Remnants, Active Galactic Nuclei, Multi-Messenger

P26**THE IMPACT OF SIFTS IN THE EARTH'S AXIS ON CLIMATE****Laura Botez**

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ABSTRACT

The orientation of Earth's rotational axis plays a fundamental role in driving both long-term geological climate shifts and short-term planetary adjustments. Historically, variations in the Earth's axial tilt (obliquity) and wobble (precession)—collectively known as Milankovitch cycles—have acted as primary catalysts for macro-level climate shifts, including the regular onset and retreat of glacial periods over thousands of years. Conversely, contemporary anthropogenic climate change has initiated a reverse feedback loop where rapid climate shifts are actively altering the Earth's rotational axis. Accelerated polar ice sheet degradation, glacier retreat, and massive global groundwater extraction have collectively redistributed trillions of tons of mass from land to the oceans. Recent geodetic observations and satellite data confirm that this substantial mass redistribution has caused a measurable shift in the Earth's geographic poles (polar motion) and minor changes in day length. This paper reviews the dual nature of this relationship, analyzing how long-term astronomical axial shifts dictate global solar radiation patterns, while modern, human-induced climate change rapidly modifies planetary rotation on a decadal scale. The synthesis highlights the critical need to integrate rotational dynamics into comprehensive global climate models to better predict future planetary responses.

Keywords: Axial Tilt, Polar Motion, Milankovitch Cycles, Climate Change, Groundwater Depletion, Geodesy.

P27**INCREASING ENERGY EFFICIENCY IN AGRICULTURE WITH ARTIFICIAL INTELLIGENCE AND SELF-GENERATING ENERGY SYSTEMS****Wang Xinyi**

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ABSTRACT

Modern agriculture faces the dual challenge of increasing food production while mitigating environmental impacts and rising operational costs. This paper investigates the integration of Artificial Intelligence (AI) and self-generating renewable energy systems—specifically solar microgrids and wind systems—to optimize energy efficiency in precision farming. We propose an intelligent edge-computing framework that leverages machine learning models for predictive weather forecasting, real-time biomass/solar yield optimization, and dynamic load-shifting. Our simulated results demonstrate that AI-driven dynamic solar tracking and smart microgrid orchestration can increase on-farm renewable energy utilization by up to 15% while reducing overall grid dependency. Furthermore, by linking AI predictive analytics with automated, solar-powered precision irrigation networks, the system achieves a 20% reduction in water waste and significantly lowers the operational carbon footprint. Ultimately, this study demonstrates that combining machine learning with localized, self-generating energy infrastructures provides a scalable pathway toward fully autonomous, climate-resilient, and sustainable agricultural ecosystems.

Keywords: Smart Agriculture, Artificial Intelligence, Self-Generating Energy, Precision Farming,

O-1**FROM MONITORING TO DECISION-MAKING: RETHINKING INDOOR AIR QUALITY ASSESSMENT IN SCHOOL BUILDINGS****Tugce PEKDOGAN^{1,*}**¹ Faculty of Architecture and Design, Department of Architecture, Adana Alparslan Turkes Science and Technology University, Adana, Turkey**ABSTRACT**

Indoor air quality (IAQ) in educational buildings has become a significant issue due to its impact on students' health, cognitive performance, and academic achievement. Advances in sensor technologies have enabled continuous monitoring of environmental parameters such as carbon dioxide (CO₂), particulate matter (PM_{2.5}), temperature, and relative humidity. As a result, schools are now able to generate large amounts of indoor environmental data. However, despite this progress, translating monitoring results into practical management decisions remains a significant challenge. Current assessment practices primarily focus on reporting individual pollutant concentrations or comparing measured values to guideline thresholds. While these approaches are necessary for regulatory compliance, they provide limited support for practical questions faced by school administrators. This study discusses the limitations of traditional IAQ assessment approaches and proposes a conceptual framework that shifts the focus from environmental monitoring to decision support. This framework emphasizes integrating temporal variability, spatial differences between classrooms, pollutant interactions, and exposure characteristics into a unified assessment perspective. In addition, highlights the need for assessment approaches that will assist facility managers and decision-makers in prioritizing interventions, allocating maintenance resources, and improving classroom environmental quality. The proposed perspective contributes to the ongoing development of IAQ assessment by bridging the gap between environmental measurements and practical building management. It also provides a foundation for future research aimed at developing decision-driven assessment methodologies for healthy and sustainable educational buildings.

Keywords: Indoor air quality, School buildings, Decision support, Environmental monitoring, Facility management**O-2****A SCENARIO-BASED SIMULATION APPROACH IN MUM-T TRAINING. THE APEX-RAMEF CASE STUDY****Vural AVCI¹**¹ Target and Friend Database Specialist / TUSAŞ - Ankara, Türkiye**ABSTRACT**

Manned-Unmanned Teaming (MUM-T) is recognized as one of the key components of next-generation air operations concepts, in which piloted platforms and autonomous or semi-autonomous unmanned aerial vehicles (UAVs) carry out joint missions. However, despite the rapid development of the MUM-T concept, simulation-based training environments that support the development of standard operating procedures (SOPs), training syllabi, and doctrine specific to this framework have not yet reached sufficient maturity. Currently, a significant portion of new operational concepts can only be validated through high-cost flight operations and complex coordination processes. This situation both extends development time and limits training activities. Therefore, there is a need for simulation environments where MUM-T missions can be modeled on the ground prior to flight and evaluated repeatedly under different scenarios.

In this study, the APEX-RAMEF (Air Planning Explorer – Real-Time Adaptive Mission Execution Framework) simulation environment, currently under development for the planning and training-oriented evaluation of MUM-T missions, is presented as a case study. The primary objective of this study is to present a simulation approach that allows piloted and autonomous platforms to be represented simultaneously within the same scenario, enables the layered tracking of mission phases, and provides situational awareness to both the instructor and the operator. In this context, the study explains the simulation environment's scenario-generation logic, platform and mission definition structure, user interface architecture, and design decisions regarding the visualization of mission flows.

The study addresses three key issues that stand out in the design of MUM-T training simulations: the simultaneous visualization of multi-layered mission phases, the maintenance of situational awareness from the perspectives of both the operator and the instructor and striking a balance between scenario flexibility and operational realism. It is demonstrated that the simulation environment developed in this context supports training and evaluation processes by presenting the tactical map, mission management, decision tree, and mission log within an integrated structure.

Consequently, it is assessed that APEX-RAMEF is not merely a simulation tool but also a development environment capable of contributing to the low-cost pre-flight testing of standard operating procedures, training syllabi, and new operational concepts for MUM-T missions. The study aims to contribute to future academic and industrial research in the fields of MUM-T training technologies, simulation-based instructional approaches, and doctrine development methodologies.

Keywords: Manned-Unmanned Teaming (MUM-T), Air Operations Simulation, Scenario-Based Simulation, Doctrine Development, APEX-RAME

O-3

PREDICTIVE MAINTENANCE OF PRODUCTION EQUIPMENT USING ARTIFICIAL INTELLIGENCE METHODS

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ABSTRACT

The work provides a comprehensive analysis of modern approaches to predictive maintenance of production equipment using artificial intelligence methods. It examines the features of reactive, preventive, and predictive maintenance strategies, as well as the principles for building predictive maintenance systems. Modern machine learning methods are analyzed, including Random Forest, LSTM, GRU, Isolation Forest, One-Class SVM, and autoencoders, highlighting their advantages, limitations, and suitability for tasks such as classifying equipment condition, predicting remaining equipment life, and detecting anomalies. The typical architecture of predictive maintenance systems has been summarized, and a comparative analysis of modern industrial predictive maintenance platforms has been carried out. Based on a review of the literature, an original qualitative comparison of machine learning methods and a generalized scheme of how predictive maintenance systems function have been developed. It was found that the effectiveness of such systems depends on a combination of quality data preparation, the choice of machine learning algorithms, and architectural decisions. The results obtained can be used as a methodological basis for designing intelligent predictive maintenance systems for production equipment in various industrial sectors.

Keywords: predictive maintenance, artificial intelligence, machine learning, methods, equipment remaining useful life prediction.

O-4

IMPROVED ALBUMIN BINDING PROPERTIES OF ISOGUVACINE UPON ESTERIFICATION

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ABSTRACT

The prevalence of epilepsy, affecting millions across all age groups, has intensified the need for novel therapeutic interventions. Despite advances in antiseizure medications (ASMs), challenges persist, particularly drug resistance and significant psychiatric and behavioral adverse effects. Isoguvacine (IGV), a potent γ -aminobutyric acid type A receptor agonist, holds promise for epilepsy treatment but suffers from poor blood–brain barrier (BBB) permeability due to its zwitterionic nature. To address this limitation, two ester prodrugs, E7 (heptyl 1,2,3,6-tetrahydropyridine-4-carboxylate) and E14 (tetradecyl 1,2,3,6-tetrahydropyridine-4-carboxylate), were synthesized to enhance BBB penetration and central nervous system (CNS) delivery. This study investigates the interactions of IGV and its derivatives with human serum albumin (HSA), a key plasma transport protein, using a suite of biophysical and computational techniques. UV spectroscopic analysis confirmed protein–ligand complexation, with E7 and E14 exhibiting enhanced binding compared to IGV. Isothermal titration calorimetry revealed that E14 demonstrated superior binding affinity ($K_a = 2.42 \times 10^6 \text{ M}^{-1}$) compared to E7 ($K_a = 3.41 \times 10^4 \text{ M}^{-1}$), while IGV showed negligible interaction. Atomic force microscopy and circular dichroism spectroscopy indicated that the enhanced hydrophobicity of E7 and E14 promoted stable protein–ligand interactions without perturbing the secondary and tertiary structures of HSA. Molecular docking studies corroborated the superior binding affinity of E14 towards HSA, while molecular dynamics simulations confirmed the enhanced stability of the E14–HSA complex. These results highlight the potential of E14 as a promising prodrug candidate for CNS-targeted epilepsy therapy and underscore the importance of albumin binding in modulating drug bioavailability and distribution.

Keywords: Isoguvacine, albumin, antiseizure medication, biomolecular interactions

O-5

EXPRESSION OF SOME QUANTITIES IN PHYSICS WITH BI-QUATERNION ALGEBRA

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ABSTRACT

The mathematical representation of fundamental physical laws often relies on separate vector calculus systems, tensor formalisms, and matrix representations to handle spacetime, electrodynamics, and quantum fields. This paper demonstrates the efficiency and structural elegance of complexified quaternions, or biquaternion algebra ($\mathbb{H}_\mathbb{C}$), as a unified hypercomplex framework capable of consolidating these disparate mathematical formulations. By mapping the eight-dimensional structure of biquaternions directly to the geometry of 4D Minkowski spacetime, we reformulate key quantities in relativistic kinematics, classical electrodynamics, and quantum mechanics. Specifically, we present the hypercomplex compression of the four Maxwell equations into a single, compact differential expression utilizing the Riemann-Silberstein field vector. Furthermore, we explore the integration of relativistic four-momentum, four-current density, and the Dirac spinor wavefunctions within this algebraic domain. Our analysis highlights how the associative multiplication of biquaternions inherently preserves Lorentz covariance and eliminates coordinate-dependent operations like dot and cross products. Ultimately, this study suggests that biquaternion algebra serves not merely as an alternative notation, but as a deeper geometric foundation that simplifies the formulation of gauge theories and provides a more intuitive pathway toward unifying classical and quantum relativistic systems.

Keywords: Biquaternions, Hypercomplex Algebra, Maxwell Equations, Minkowski Spacetime, Relativistic Quantum Mechanics, Lorentz Covariance.

O-6

VIRTUAL PHYSICS COURSE LAB APPLICATIONS (VPCLApps): DESIGN AND IMPLEMENTATION OF INNOVATIVE DIGITAL LEARNING ENVIRONMENTS IN PHYSICS EDUCATION

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ABSTRACT

Digital transformation has become a major priority in European education policies, particularly through the European Commission's *Digital Education Action Plan 2021–2027* and the Erasmus+ horizontal priority of Digital Transformation. In line with these priorities, the Erasmus+ KA220-SCH project "Virtual Physics Course Lab Applications (VPCLApps)" (Project No. 2023-2-TR01-KA220-SCH-000178323) aims to support physics education through innovative and accessible digital learning environments. The project develops three complementary educational outputs: a Virtual Physics Laboratory with desktop and virtual reality applications, a Digital Physics E-book combining theoretical knowledge with step-by-step experimental activities, and a Teacher Toolkit supporting the pedagogical integration of these resources. Through interactive virtual experiments, students can explore physics concepts, manipulate variables, collect and analyse data, and connect theoretical knowledge with experimental processes. VPCLApps therefore contributes to technology-enhanced, learner-centred physics education while supporting the European Union's objectives for accessible, inclusive, and digitally supported learning.

Keywords: Virtual Physics Laboratory, VPCLApps, Digital Education, Virtual Reality, Physics Education, Digital Transformation

O-7

A DIALOGUE-BASED DECISION-MAKING SYSTEM FOR SOLVING PLANNING PROBLEMS UNDER UNCERTAINTY

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ABSTRACT

Decision-making process is characterized by the need to resolve complex, multi-criteria issues. Decisions in fields such as economics, logistics, healthcare, industry, and public administration are frequently made under conditions of uncertainty. The incomplete, imprecise, or volatile nature of data directly impacts the quality of these decisions. In this context, dialogue-based decision-making systems create opportunities for more efficient planning by combining the user's knowledge and experience with intelligent algorithms. This article examines the application of dialogue-based decision-making systems for solving planning problems under conditions of uncertainty. In modern intelligent systems, the processing of uncertain data, the management of user interaction, and the making of optimal decisions are of significant importance. Dialogue systems facilitate interactive collaboration with the user to evaluate various alternatives, analyze risks, and ensure the selection of the most suitable decision. The article analyzes the design principles, advantages, and application areas of such systems.

Keywords: decision-making, dialogue system, uncertainty, planning, artificial intelligence, expert system.

O-8

ANALYSIS OF QUADRUPOLE MOMENT OF ATOMIC NUCLEUS WITH OCTONIONS

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ABSTRACT

Assuming a prolate spheroid nucleus, this allows to quantify the sensitivity of the nuclear transition frequency to variations of the finestructure constant α to $K = 5800$ (2100), with the uncertainty dominated by the experimentally measured charge radius difference $\Delta\langle r^2 \rangle$ between the ground and isomeric state. This result indicates a three orders of magnitude enhancement over atomic clock schemes based on electron shell transitions. In this study we will explain this station.

O-9

CHARACTERIZATION OF AlGaSb NANOCRYSTALLINE PRODUCED BY MECHANICAL

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ABSTRACT

In this study, ternary nanocrystalline aluminium gallium antimonide $\text{Al}_x\text{Ga}_{1-x}\text{Sb}$ alloys were successfully synthesized via high-energy mechanical alloying (MA) from elemental Al, Ga, and Sb powder mixtures. The effect of mechanical milling duration on the structural evolution, phase transformation, morphology, and optical properties of the synthesized powders was systematically investigated. X-ray diffraction (XRD) analyses revealed that the individual elemental phases gradually disappeared, transforming completely into a single-phase cubic zinc-blende ternary structure after progressive milling hours. The average crystallite size was refined down to the nanoscale 10–25 nm, accompanied by a significant increase in internal microstrain due to cumulative lattice distortions and severe plastic deformation. Scanning electron microscopy (SEM) observations tracked the morphological transition from irregular, fractured flakes to highly homogenous, agglomerated submicron composite particles. Furthermore, UV-Vis diffuse reflectance spectroscopy demonstrated that the optical bandgap of the nanostructured $\text{Al}_x\text{Ga}_{1-x}\text{Sb}$ could be effectively tuned by varying both the milling duration and the Al-to-Ga composition ratio x . These findings suggest that solid-state mechanical alloying is a robust, scalable route for tailoring the structural and electronic parameters of $\text{Al}_x\text{Ga}_{1-x}\text{Sb}$ nanocrystals for advanced optoelectronic and thermoelectric applications.

Keywords: Mechanical alloying, Nanocrystalline materials, $\text{Al}_x\text{Ga}_{1-x}\text{Sb}$, X-ray diffraction, Semiconductor synthesis, Bandgap engineering.

O-10

MICROBIAL NANOBIO TECHNOLOGY FOR GREEN SYNTHESIS OF SILVER NANOPARTICLES: SCREENING, CHARACTERIZATION, AND ASSESSMENT OF ANTIFUNGAL ACTIVITY

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ABSTRACT

Microbial nanobiotechnology, or microbial nanotechnology, is a rapidly developing field that has emerged in the 21st century. It focuses on the development of nanoscale materials, typically ranging from 1 to 100 nanometers (nm), which are of significant scientific and commercial interest. This study aimed to investigate the green synthesis of silver nanoparticles (AgNPs) from silver nitrate using bacterial isolate *Brevibacillus parabrevis* OW4. Initially, the ability of these isolate to biosynthesize AgNPs was screened. The resulting nanoparticles were then characterized and evaluated for their antifungal activity. AgNPs were synthesized using bacterial cell-free filtrate (CFF) under controlled conditions. The synthesized nanoparticles were characterized using UV-Vis, FT-IR, XRD, FESEM, and EDX. Antifungal activity of the AgNPs was examined against *Nakaseomyces glabrata* (*Candida glabrata*), *Pichia kudriavzevii* (*Candida krusei*), and *Candida albicans* using disk diffusion, agar well diffusion, and microdilution methods.

The results demonstrate that the cell-free filtrate (CFF) of the *B. parabrevis* OW4 successfully generated biogenic AgNPs. The green synthesis of silver nanoparticles exhibited a strong surface plasmon resonance peak at 425 nm, with a spherical shape. The AgNPs showed high antifungal activity against the tested strains. These findings support the potential use of biosynthesized AgNPs from *B. parabrevis* OW4 as effective antimicrobial agents.

Keywords: Green synthesis, silver nanoparticles, nanotechnology, Antifungal activity.

O-11

A SEMI-SUPERVISED LEARNING APPROACH FOR SEGMENTATION OF RAILWAY TRACKS AND STRUCTURAL HEALTH MONITORING

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ABSTRACT

The maintenance of railway tracks is essential for the sustainability of transportation systems and to prevent accidents. While conventional visual inspection methods can lead to fatigue and human-dependent errors, fully supervised deep learning-based artificial intelligence models demand significantly high data labeling expenses. The objective of this investigation is to create a semi-supervised semantic segmentation architecture that considers geometry, which will automate the inspection processes of railway tracks and reduce labeling expenses. The main feature of the proposed model is its ability to provide high-precision learning with a small amount of labeled data by teaching the network the perspective narrowing and the parallelism of each track as essentially 'a mathematical constraint' (Geometric Loss). Skeletonization algorithms are applied to the track masks of the architecture to enable the detection of structural anomalies through an independent decision support module. Thus, the objective of this project is to create an innovative and cost-effective digital infrastructure for railway structural health monitoring systems that is both robust and resilient against harsh environmental conditions and free from human error.

Keywords: Railway Safety, Semi-Supervised Learning, Semantic Segmentation, Geometric Loss, Structural Health Monitoring

O-12

DETERMINING THE FINANCIAL BEHAVIOR PROFILES OF CONSTRUCTION INSPECTION STUDENTS USING DECISION TREES AND CLUSTER ANALYSIS

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ABSTRACT

The increase in average life expectancy, demographic changes in society, and the diverse behavioral characteristics of individuals are creating global pressure on the sustainability of traditional public social security systems, a pressure that also significantly affects Turkey. To alleviate this pressure and achieve the macroeconomic fund accumulation goal underlined in the 12th Development Plan, the government and public authorities are implementing various tools. The individual retirement system and its extension, the automatic enrollment system, are particularly aimed at encouraging young people to develop saving habits at an early age. This study, contrary to the general trend in the literature, investigates the financial tendencies of students in a technical associate degree program. The main objective of this study is to reveal the structural financial behavior profiles of associate degree students by analyzing their participation tendencies in the retirement system, their knowledge levels, and their trust attitudes towards the system using machine learning algorithms. In the analysis of the dataset, decision tree algorithms were used to create a predictive model, and hierarchical clustering algorithms were used to divide students into homogeneous financial groups. The findings from the decision tree analysis show that the most dominant determinant of students' decision to participate in the individual retirement system is household income. Furthermore, findings showed that construction supervision students in the lower-middle income group differed dramatically from the control group. Hierarchical clustering analysis revealed that the students were divided into three distinct financial profiles. These findings have the potential to contribute to the development of specific policy interventions based on behavioral finance.

Keywords: Financial Literacy, Decision Trees, Clustering Analysis, Retirement System.

O-13

ENERGETIC AND MECHANISTIC INSIGHTS INTO CHEMICAL REACTIONS OF THE DISULFIDE BOND IN DIMETHYL DISULFIDE: A THEORETICAL APPROACH

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France

ABSTRACT

The covalent disulfide (S–S) bond plays a pivotal role in biochemical pathways, polymer chemistry, and atmospheric processes. In this study, we provide comprehensive energetic and mechanistic insights into the chemical reactions of dimethyl disulfide CH_3SSCH_3 , DMDS—the primary prototype for S–S bond dynamics—utilizing advanced quantum chemical calculations. Thermal decomposition, radical-induced oxidation OH^* photodissociation, and nucleophilic thiolate-disulfide exchange pathways were systematically investigated using Density Functional Theory (M06-2X, B3LYP) and high-level composite methods (CBS-QB3, MS-CASPT2). Our calculations reveal that thermal decomposition is governed by homolytic S–S bond scission, transitioning through key dithiirane and thioformaldehyde intermediates. Under atmospheric conditions, the reaction with OH^* radicals preferentially follows an O–S coupling addition pathway, forming a transient CH_3SSCH_3 intermediate with a near-collision-limited rate constant. Multi-reference excited-state simulations mapping the near-UV photodissociation confirm an ultrafast repulsive repulsive pathway leading to thiyl radical production. Furthermore, solvent-corrected nucleophilic attacks demonstrate a classic $\text{S}_\text{N}2$ like substitution mechanism featuring a localized trisulfur anionic transition state. These theoretical findings clarify the fundamental electronic factors governing disulfide reactivity, offering robust parameters for modeling complex sulfur chemistry across biological and industrial systems.

Keywords: Dimethyl disulfide, S–S bond scission, Quantum chemistry, Reaction mechanism, Thermal decomposition, Ab initio calculations.

O-14

EFFECTS OF DATA SPLITTING STRATEGIES ON RECOMMENDER SYSTEM EVALUATION**Ömer ŞENTÜRK¹, Zeynep BATMAZ^{1*}**¹ Computer Engineering Department, Faculty of Engineering, Eskişehir Technical University, Eskişehir, Türkiye**ABSTRACT**

Offline evaluation is widely used to compare recommender systems, but its results can change with the selected data splitting strategy. Earlier studies showed that split choice, temporal leakage, random seeds, and sampling can change accuracy and model rankings. However, most studies examine a limited set of model families, focus mainly on accuracy, or study a single domain or recommendation task. They rarely compare traditional, deep learning, and graph-based methods in the same software environment while also considering dataset density and computational cost. This study addresses this research problem by evaluating nine algorithms with a ratio split, a user based stratified split, and 5-fold cross-validation. The experiments use the relatively dense MovieLens-100K dataset and a sparse Amazon-Toys subset. Accuracy is measured with normalized discounted cumulative gain at 10 (NDCG@10), Precision@10, Recall@10, and F1@10. Both training and test times are also reported. On MovieLens-100K, the Multi-Layer Perceptron with five-fold cross-validation gives the highest NDCG@10 value of 0.2153. On Amazon-Toys, Neural Graph Collaborative Filtering with the ratio split gives the highest NDCG@10 value of 0.0446. The findings show that the best split depends on the algorithm and dataset. 5-fold cross validation often improves ranking accuracy, especially on the sparse dataset, but the ratio split and stratified split also produce the best results for some algorithms. 5-fold cross validation also increases total runtime because each algorithm is trained and tested five times. Therefore, data splitting should be treated as a main part of recommender system evaluation rather than a minor implementation choice.

Keywords: Data splitting, recommender systems, offline evaluation, accuracy, computational cost

O-15

MOS AND WSE MONOLAYERS AS ANODE MATERIALS ELECTRIC FIELD EFFECT**Abdullah Ensarit**

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ABSTRACT

Two-dimensional (2D) transition metal dichalcogenides (TMDs) have emerged as highly promising anode materials for next-generation alkali-metal-ion (Li⁺, Na⁺, and K⁺) batteries due to their large surface-to-volume ratios and unique electronic properties. In this work, we employ first-principles density functional theory (DFT) calculations to systematically investigate the adsorption, diffusion, and storage capacities of Li, Na, and K ions on monolayer MoS₂ and WSe₂, with a particular focus on the modulation effects of a perpendicular external electric field (E-field). Our results demonstrate that both monolayers exhibit strong binding affinity and favorable structural stability upon ion intercalation, yielding high theoretical storage capacities. Specifically, monolayer MoS₂ delivers exceptional capacities of 1,674.32 mAh/g for Li and 1,339.46 mAh/g for Na, while WSe₂ exhibits stable low-voltage storage capabilities. Crucially, the application of a perpendicular electric field ranging from 0 to 0.8 V/Å acts as a powerful tool to tune the electronic structure and charge transfer at the interface. The external field significantly reduces the minimum diffusion energy barriers for the adatoms, thereby drastically accelerating ion mobility and improving rate capability. These findings highlight the critical role of external field engineering in overcoming kinetic limitations, positioning MoS₂ and WSe₂ monolayers as highly controllable, ultra-fast charging anode materials for high-performance alkali-metal-ion batteries.

Keywords: metal dichalcogenides, anode materials, unique electronic properties.

O-16

INCREASING THE EFFICIENCY OF THE THERMOGRAPHIC TECHNIQUES FOR EARLY DIAGNOSTICS OF THE TRANSFORMER CONDITION**Volodymyr STOROZHENKO, Sergiy MESHKOV, Oleksandr MIAHKYI, Roman OREL**

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ABSTRACT

The power supply system is considered critical infrastructure, and a significant portion of it relies on the operation of transformer systems. Rapid transformer diagnostics help maintain this system in good working order and prevent failures. The rapid transformer diagnostics aims to identify devices with increased electrical discharge activity and thermal anomalies at an early stage, and to plan their decommissioning at critical parameters. To achieve this aim, a thermographic method for early diagnostic of transformer condition is used, based on a comparison of the thermographic information function (TIF) of the object under study and the TIF standard.

This method implements the following functions:

- analyzes the uploaded image and generates a TIF based on it in the specified temperature range, with a graphical display of the results;
- generates a “standard” TIF based on the submitted images, with a graphical display of the results,
- compares the TIF of the object being studied with the TIF of the standard,
- evaluates the coefficient used to assess the technical condition of the transformer,

At the same time, the results of this method are distorted by the inclusion of objects structurally unrelated to the unit in the frame. The effectiveness of this method can be improved by removing these extraneous elements from the corresponding thermograms (Fig. 1) using a technique developed by the authors based on image processing.

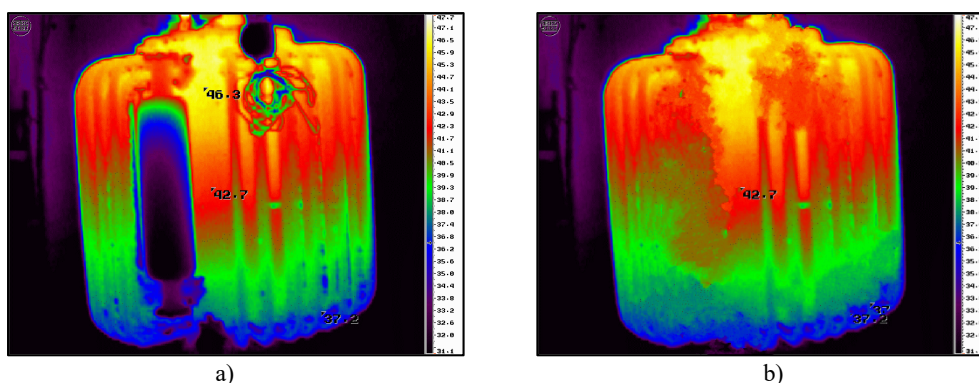


Fig. 1. Thermographic image of the transformer before (a) and after (b) processing.

Eliminating extraneous elements from the thermogram gives the possibility to significantly increase the accuracy of the TIF by 18% and improve the reliability of the method by 12%.

The optimized method enables efficient analysis of transformer thermograms, comparison with a standard, and rapid equipment evaluation. This simplifies the operation of power systems and prevents emergencies.

Keywords: Transformers, Thermographic method, Reference information function, Thermogram processing

O-17

PHOTOISOMERIZATION AND CONFORMATIONAL ANALYSIS OF MATRIX-ISOLATED PHTHALIC ACID

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ABSTRACT

Matrix isolation experiments of phthalic acid (PA) in argon at 15 K allowed the investigation of its conformational landscape and photochemical behavior. The PA₁ conformer was trapped as the predominant species, exhibiting well-resolved IR bands in excellent agreement with DFT-calculated vibrational frequencies. Relative energies calculated at the B3LYP/6-311++g(d,p) level indicated PA₁ as the most stable conformer (0.0 kJ·mol⁻¹), PA₂ slightly less stable (+0.7 kJ·mol⁻¹), and PA₃ as the least stable (+2.85 kJ·mol⁻¹). Upon IR/NIR irradiation at 6974 cm⁻¹ for 10 minutes, PA₂ and PA₃ conformers were generated, demonstrating the photochemical flexibility of PA. These findings provide insight into the structural dynamics and photoinduced transformations of PA under isolated conditions.

Keywords: Matrix-isolation, DFT calculation, Phthalic acid, IR/NIR irradiation.

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O-18

DECENTRALIZED IDENTITY VERIFICATION USING BLOCK CHAIN

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ABSTRACT

Organizations and individuals are confronted with increasing issues with data protection, identity verification, and fragmented systems as the digital world quickly changes. By granting consumers complete control over their data and facilitating safe and easy cross-platform interactions, decentralized identification technology solves these problems. Dock has been in the forefront of developing cutting-edge decentralized identification and verified credential solutions since 2017, assisting companies in overcoming these contemporary obstacles. Decentralized identity employs tamper-proof, cryptographically secured digital credentials kept in a user-controlled ID wallet, in contrast to traditional centralized systems that experience fraud, sluggish onboarding, and frequent data breaches. People can safely and carefully manage and exchange their identification information using these wallets. Verifiable credentials and ID wallets are the two main pillars of the decentralized identity ecosystem, which together guarantee security, openness, and user autonomy. Reusable digital identities for onboarding, supply chain traceability, issuing tamper-proof certificates, and maintaining employee credentials are just a few of the fast growing applications of this technology today.

Keywords: Decentralized identity, Data privacy, Identity verification, Fragmented systems, User control, Secure interactions, Dock, Verifiable credentials, ID wallet, Cryptographically secured, Tamper-proof credentials, Onboarding, Data breaches, Supply chain traceability, Digital certifications, Employee credentials

O-19

MACHINE LEARNING PREDICTION OF BAND GAPS IN ABX₃ PEROVSKITES USING OPEN MATERIALS DATABASES AND COMPOSITION-BASED FEATURES**Muhammet ARUCU^{1,*}, Ahmet AKKAYA¹**¹ Department of Computer Technologies, Bandırma Onyedi Eylül University, Gönen, Türkiye**ABSTRACT**

Accurate knowledge of the electronic band gap is essential for the rational design of semiconductors used in photovoltaic and optoelectronic devices; however, first-principles calculations based on density functional theory (DFT) are computationally expensive when large chemical spaces must be screened. In this study, a machine learning framework that predicts the band gaps of ABX₃ perovskite compounds directly from their chemical composition is presented, without performing any new electronic structure calculations. A dataset of 1798 unique perovskite-type compositions (942 semiconductors/insulators and 856 metals), together with their DFT-computed band gaps, is retrieved from the open-access Materials Project database, and only the thermodynamic ground-state polymorph of each composition is retained in order to eliminate duplicate-composition noise and data leakage. For each compound, 148 composition-based descriptors, including elemental electronegativity, covalent radii, valence electron statistics, and melting temperatures, are generated using the matminer featurization library. Linear (Ridge) and ensemble-based (Random Forest and Gradient Boosting) regression models are trained and compared using five-fold cross-validation. The hyperparameter-optimized Gradient Boosting model achieves a mean absolute error of 0.56 eV and a coefficient of determination of 0.74, and permutation importance analysis reveals that the fraction of d valence electrons is the dominant descriptor, consistent with the role of transition-metal d states in defining the band edges of perovskites. The results demonstrate that open-database-driven machine learning is a practical and computationally inexpensive screening tool for the discovery of candidate perovskite absorbers in energy applications. All calculations are implemented in Python using open-source libraries.

Keywords: Machine learning, band gap prediction, perovskites, Materials Project, computational physics

O-20

SUSTAINABLE AND GREEN ORGANIC CATALYST TECHNOLOGIES FOR NEXT-GENERATION FUEL CELLS**Arif KIVRAK^{1,*}, Hilal DEMİR KIVRAK²**¹Eskişehir Osmangazi University, Faculty of Science, Department of Chemistry, 26040, Eskişehir, Türkiye²Eskişehir Osmangazi University, Faculty of Engineering and Architectural Sciences, Department of Chemical Engineering, Eskişehir, Türkiye
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The increasing global energy demand and the environmental challenges associated with fossil-fuel dependence necessitate the development of sustainable and efficient energy conversion technologies. Fuel cells represent a promising alternative for clean energy generation; however, the widespread application of fuel cell technologies remains strongly dependent on the development of efficient, economically viable, and environmentally sustainable electrocatalysts. In this context, the development of metal-free catalytic systems offers an attractive strategy for reducing dependence on conventional metallic catalyst materials and improving material sustainability.

In this study, a series of organic and heterocyclic compounds, including indole-, benzofuran-, thymol-, pyrazole-, and carbazole-based structures, were designed, synthesized, and characterized as potential metal-free anode electrocatalysts for fuel cell applications. Their electrochemical properties and catalytic performances were systematically investigated through hydrazine and glucose electrooxidation reactions. The relationship between molecular structure and electrochemical activity was evaluated to identify structural features contributing to enhanced anodic catalytic performance.

The results demonstrate that the synthesized organic frameworks exhibit promising electrochemical and electrocatalytic properties, highlighting their potential as tunable alternatives to conventional metal-based catalyst systems. In addition to their catalytic performance, the use of metal-free organic materials provides potential advantages in terms of resource efficiency, material sustainability, cost reduction, and reduced reliance on critical metallic elements. These characteristics are particularly relevant to the development of environmentally compatible and sustainable energy conversion technologies.

Overall, our results demonstrate that organic electrocatalysts can contribute to the development of next-generation fuel cell systems and support the transition toward cleaner, resource-efficient, and low-carbon energy technologies. The study provides a molecular-level approach to sustainable electrocatalyst development and highlights the potential of metal-free organic materials for advancing sustainable fuel cell technologies.

Keywords: Heteroaromatic Compounds, Energy, Fuel Cell, Renewable Energy

O-21

THEORETICAL INVESTIGATION OF THE STRUCTURAL, ELECTRONIC, AND VIBRATIONAL PROPERTIES OF 8-CHLOROTHEOPHYLLINE USING DFT AND TD-DFT METHODS

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ABSTRACT

8-Chlorotheophylline is a xanthine derivative of considerable pharmaceutical importance due to its application in medicinal chemistry and drug formulations. In this study, the structural, electronic, and vibrational properties of 8-chlorotheophylline were theoretically investigated using Density Functional Theory (DFT) and Time-Dependent Density Functional Theory (TD-DFT). All calculations were carried out at the B3LYP/6-311++G(d,p) level of theory. The optimized molecular geometry was confirmed as a true minimum by the absence of imaginary vibrational frequencies. Geometrical parameters and vibrational frequencies were analyzed to characterize the molecular structure and identify the fundamental vibrational modes.

The electronic properties of the molecule were examined through frontier molecular orbital (HOMO–LUMO) analysis, and quantum chemical descriptors such as the energy gap, ionization potential, electron affinity, chemical hardness, softness, electronegativity, and electrophilicity index were determined. In addition, Molecular Electrostatic Potential (MEP) analysis was performed to identify the most probable reactive regions of the molecule. The electronic absorption spectrum was investigated using TD-DFT calculations, and the main electronic transitions were interpreted in terms of excitation energies, oscillator strengths, and orbital contributions. The theoretical results provide a comprehensive understanding of the molecular structure, stability, electronic behavior, and spectroscopic properties of 8-chlorotheophylline, offering useful reference data for future experimental and pharmaceutical studies.

Keywords: 8-Chlorotheophylline; Density Functional Theory (DFT); Time-Dependent Density Functional Theory (TD-DFT); Molecular Electrostatic Potential (MEP); HOMO–LUMO Analysis..

O-22

TRANSFER MATRIX ANALYSIS OF ONE-DIMENSIONAL PHOTONIC CRYSTALS: DESIGN OF BRAGG REFLECTORS AND DEFECT-MODE OPTICAL FILTERS

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ABSTRACT

One-dimensional photonic crystals, consisting of periodically alternating dielectric layers, exhibit photonic band gaps in which the propagation of light is forbidden, and they form the basis of high-reflectivity mirrors, optical filters, and sensing platforms. In this work, the optical response of one-dimensional photonic crystal structures is investigated numerically by means of the transfer matrix method (TMM) implemented entirely in Python using open-source libraries. The implementation is verified against four independent analytic results, including the exact single-film reflectance formula, with agreement at machine precision (deviations below 10^{-16}). Quarter-wave SiO₂/TiO₂ Bragg reflectors centered at 550 nm are then designed: the computed photonic stopband of 477–649 nm agrees with the analytic coupled-band expression to within 1%, and the peak reflectance reaches 99.88% for 8 bilayers and 99.998% for 12 bilayers. The angular and polarization dependence of the stopband is mapped, and the reflectance spectra are connected to the Bloch band structure of the infinite crystal. Finally, a half-wave defect layer embedded in the mirror is shown to open a sharp Fabry-Perot resonance inside the stopband with a quality factor of about 1100, a resonant field enhancement of 207 inside the defect, and a spectral position tunable between 480 and 598 nm through the defect thickness. The quality factor grows exponentially with the mirror size, by a factor of 2.75 per added bilayer, and filling the defect with an analyte yields a refractometric sensitivity of 168 nm per refractive index unit, demonstrating that the presented open-source TMM framework is an efficient design tool for narrow-band optical filters and photonic sensor structures.

Keywords: Photonic crystals, transfer matrix method, Bragg reflector, defect mode, optical filter

O-23

NANOPOROUS METAL OXIDE THIN FILMS VIA SOFT TEMPLATING

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ABSTRACT

Transparent nanoporous metal oxide thin films possessing controlled morphology, high structural uniformity, and large-area coverage have attracted significant attention owing to their broad potential in sensing, optoelectronics, photocatalysis, energy conversion, and as functional templates for advanced materials, including metal–organic frameworks (MOFs). However, many existing fabrication techniques involve complex, costly, or multistep procedures, underscoring the demand for straightforward, scalable, and cost-effective synthesis routes. Among the available approaches, lyotropic liquid crystal (LLC) templating has emerged as a particularly promising soft-templating strategy, enabling the one-pot fabrication of highly ordered nanoporous metal oxide thin films with tunable nanostructures over large areas under relatively mild processing conditions.

Keywords: Soft templating, nanoporous materials, transparent thin films, metal oxide, lyotropic liquid crystal, liquid crystal templating

O-24

ECO-FRIENDLY SYNTHESIS AND CHARACTERIZATION OF SILVER-COATED SILICON DIOXIDE NANOCOMPOSITES USING HYPERICUM PERFORATUM L.

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ABSTRACT

Silver nanoparticles (AgNPs) have attracted considerable attention due to their potential applications in areas such as catalysis, food packaging, water disinfection, drug delivery, and antimicrobial coatings. However, AgNPs are sensitive to environmental factors such as heat, light, and pH, which may lead to a decrease in their effectiveness over time. Therefore, many researchers have used matrices such as zeolite, clay, alumina, and silica to develop silver-containing antimicrobial agents. In this study, silver-coated silicon dioxide (AgNP-SiO₂) nanocomposites were synthesized using a novel green synthesis method and characterized. In this synthesis approach, an oil-based extract prepared from *Hypericum perforatum* L. (St. John's wort) was used, and Ag nanoparticles were formed through the reduction of Ag⁺ ions at room temperature using an economical method. In the UV-Vis analyses of the obtained nanocomposites, a characteristic surface plasmon resonance absorption band supporting the formation of Ag nanoparticles was observed in the range of approximately 373–404 nm. In the FTIR analyses, the bands observed at approximately 2854, 2926, 1711, and 1467 cm⁻¹ were attributed to C–H stretching and bending vibrations, indicating the presence of organic components originating from St. John's wort. The peaks observed at 1060 and 808 cm⁻¹ corresponded to the characteristic asymmetric and symmetric Si–O–Si stretching vibrations of the SiO₂ structure, respectively. The weak vibration observed at 727 cm⁻¹ was attributed to Ag–O lattice vibrations. According to the TEM images, the average size of the AgNPs was calculated as 20.61 ± 7.37 nm. XRD analyses indicated that the obtained nanocomposites generally exhibited an amorphous structure. TGA analyses revealed approximately 5% water loss at 50 °C and approximately 12% degradation of organic components occurring between approximately 200 and 500 °C. Thus, the FTIR and TGA results together indicated the presence of functional organic components associated with the surface of the synthesized AgNP-SiO₂ nanocomposites. These novel nanocomposites, synthesized through an economical and environmentally friendly method, have considerable potential for use in various important applications.

Keywords: Silver nanoparticles, *Hypericum Perforatum* L., Nanocomposites, Synthesis

O-25

PROMOTER OR POISON? THE EFFECT OF ZnO STABILITY ON CATALYTIC ACTIVITY IN AMINE-ASSISTED CO₂ HYDROGENATION TO METHANOLMuhammad Zeeshan-Asad,^a James C. Reynolds,^a Sandra E. Dann^a and Simon A. Kondrat^{a*}^aDepartment of Chemistry, Loughborough University, LE11 3TU, UK

ABSTRACT

Methanol synthesis from amine-captured CO₂ involves a key mechanistic step in which formate is converted into formamide, a process previously reported to be accelerated by a heterogeneous ZnO promoter. In this study we investigate how ZnO stability under Ru-MACHO catalysed reaction conditions influences catalytic performance. Under nearly all reaction conditions studied, and irrespective of whether dimethylethylenediamine (DMEDA) or pentaethylenhexamine (PEHA) was used, ZnO was found to dissolve completely in the polar ammonium-carbonate/formate product layer. When using PEHA, electrospray ionisation mass spectrometry identified cationic [Zn-PEHA]²⁺ complexes (base peak at m/z 148.0830 with a distinctive isotopic pattern indicative of Zn) which strongly bound formate reaction intermediates. As a result, methanol TON decreased from 607 Ru⁻¹ to 118 Ru⁻¹, 101 Ru⁻¹ and 89 Ru⁻¹ on the addition of 20, 40 and 60 mg ZnO respectively, equating in the case of 20 mg ZnO to an 80 % decrease in TON. A similar 61% decrease in TON was observed when DMEDA was used. Only when mixing between the ammonium-carbonate layer and ZnO was minimised through reduction in reaction volume or stirring rate could a solid Zn phase be recovered and catalytic activity modestly promoted (at 48 h the methanol TON of 780 Ru⁻¹ was observed with ZnO vs 531 Ru⁻¹ without). However, even under these conditions ZnO stability was found to be limited with post reaction analysis revealing partial conversion of ZnO into Zn₄CO₃(OH)₆·4H₂O formed from solvated Zn²⁺ ions reacting with the CO₃²⁻ in solution. The results demonstrate that while heterogeneous ZnO may increase catalytic turnover (i.e. through promoter behaviour), its solubilisation leads to a catalytic performance that decreases beyond the baseline activity without ZnO (i.e. a poison). The findings underscore the potential and challenges of combining homogeneous and heterogeneous catalysis to influence the complex mechanistic pathways involved in combined amine-CO₂ capture and hydrogenation process.

Keywords: Amine assisted CO₂ hydrogenation, ZnO promoter, ZnO stability, biphasic amine CO₂ capture, Ru- MACHO-BH

O-26

DETERMINATION OF THE REGULATORY ROLE OF *CATHARANTHUS ROSEUS* L. ON GLUCOSE METABOLISM AND ADIPOCYTE FUNCTIONS IN 3T3-L1 ADIPOCYTE CELLS

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Catharanthus roseus is a significant medicinal plant recognized for its antioxidant, anti-inflammatory, and metabolic regulatory effects, primarily due to its terpenoid indole alkaloids, flavonoids, and phenolic compounds. Prior research has shown that certain alkaloids found in this plant can stimulate the AMPK and AKT signaling pathways, which are crucial for the management of cellular energy metabolism. The activation of these pathways has been linked to the movement of GLUT4 vesicles to the plasma membrane, subsequently boosting cellular glucose uptake. New findings additionally indicate that *C. roseus* may have a regulatory impact on glucose metabolism and adipocyte functionality.

The current research aimed to assess the cytotoxic effects of ethanol extract from *C. roseus* on the 3T3-L1 preadipocyte cell line, identify a suitable sublethal concentration for further molecular analyses, and explore the expression of genes linked to adipocyte function, energy balance, and mitochondrial regulation. Cell viability was evaluated through the MTT assay after treating the cells with various concentrations of the extract over incubation periods of 24 and 48 hours. The results indicated that, after 24 hours of incubation, cell viability was similar to that of the control group for all concentrations tested. However, after 48 hours of exposure, the extract demonstrated a dose-dependent cytotoxic effect, particularly at concentrations of 25 and 50 µg/mL, where a marked decrease in cell proliferation was noted. In contrast, treatment with 12.5 µg/mL maintained both cell viability and the integrity of cellular morphology.

In conclusion, the 12.5 µg/mL concentration of *C. roseus* extract was identified as a suitable sublethal dose for investigating cellular and molecular effects without inducing toxicity. Accordingly, this concentration was selected for subsequent gene expression analyses related to adipocyte function, energy balance, and mitochondrial regulation, and investigations of the relevant genes have been initiated.

Keywords: *Catharanthus roseus*, 3T3-L1, MTT, cytotoxicity, adipogenesis

O-27

COMMUNITY STRUCTURE AND TEMPORAL DYNAMICS OF VESPID WASPS (HYMENOPTERA: VESPIDAE) IN A MALAYSIAN SECONDARY FOREST

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ABSTRACT

Vespid wasps are ecologically important insects that contribute to ecosystem functioning through predation of arthropod pests, pollination, and nutrient cycling. Despite their ecological significance, information on the diversity and community structure of Vespidae in Malaysian secondary forest ecosystems remains scarce. This study investigated the diversity, abundance, and temporal distribution of vespid wasps in Bukit Rupa, Universiti Kebangsaan Malaysia (UKM), to establish baseline data for biodiversity assessment and conservation. Sampling was conducted over five months (October 2024–February 2025) using three Malaise traps with weekly collections. Specimens were identified to genus or morphospecies level, and community structure was evaluated using the Shannon–Wiener diversity index (H'), Margalef species richness (R'), and Pielou's evenness index (E') in PAST software. A total of 101 individuals representing three subfamilies and 10 morphospecies were recorded. Polistinae was the dominant subfamily (59 individuals), followed by Eumeninae (27) and Vespinae (15). *Ropalidia stigma* was the most abundant species, whereas *Eumenes* sp. 4 was represented by a single individual. Temporal variation in abundance was evident, with the highest number of individuals collected in November ($n = 38$) and the lowest in February ($n = 12$). Species diversity was highest in November ($H' = 1.953$), while the greatest species richness was recorded in January ($R' = 2.299$), suggesting increased morphospecies turnover during this period. The highest evenness occurred in February ($E' = 0.938$), indicating a more balanced distribution of individuals among species despite lower overall abundance. These findings demonstrate that Bukit Rupa supports a moderately diverse vespid community with distinct seasonal variation in community structure. The study provides valuable baseline information for long-term monitoring of Hymenoptera diversity and highlights the importance of conserving fragmented forest habitats as reservoirs of beneficial insect biodiversity.

Keywords: Vespidae, Diversity, Secondary Forest, Malaise trap

O-28

APPLICATION OF THERMOGRAPHY TO MONITOR PIPELINES LOCATED IN THE SOIL

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ABSTRACT

It is known that a pipeline buried in the soil, when transporting a substance with a temperature different from the soil temperature, is a source of heat and creates a temperature anomaly on the soil surface, which can be recorded by special devices (thermal imagers, radiometers). Many pipeline defects (leaks, blockages, and damaged thermal insulation) also act as additional heat sources, creating additional temperature fluctuations. Using thermographic methods to analyze temperature fields can help decipher the internal structure of the test object, identify heat sources, and their characteristics.

To achieve this goal, the authors constructed a thermophysical model of a pipeline with defects, analyzed the factors influencing the temperature distribution over the pipeline, developed thermography techniques, and provided recommendations for reducing environmental impacts.

The principle of thermographic inspection of an underground pipeline is illustrated in Figure 1. The heat generated by the pipeline creates a temperature profile on the soil surface, which is recorded by a thermal imager (TI).

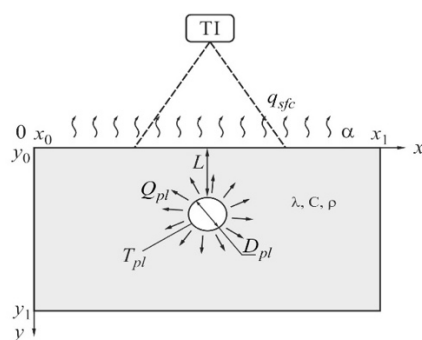


Fig. 1. Scheme of thermographic inspection of the pipeline

It has been established that the excessive temperature of the soil surface above the pipeline can be several degrees, and the temperature anomaly caused by the leakage of the substance is 2-3 times greater, which is sufficient to identify the locations of pipelines and defects in them, as well as to determine their parameters.

Based on this model, a control method was developed that includes thermogram analysis, recognizing the depth of pipeline location, finding the defect (leak), and evaluating its parameters. The influence of natural factors on the measurement results – solar radiation, heterogeneity of soil parameters – is considered, and measures to reduce errors are proposed. Practical testing of the developed methodology was conducted on a real gas pipeline at an oil and gas field. The pipeline's depth was determined to be 1 meter, with an error of 1 to 20% depending on environmental conditions. It has been shown that the thermography method can detect leaks of liquid products with an energy reserve of 42106 Joules/hour. It is equivalent to 0.5 m³/hour of water, with a temperature difference between the substance and the environment of at least 20 °C.

Keywords: Thermography, Pipelines in the ground, Depth of the location, Leaks detection

O-29

PHYSICS COURSE VIRTUAL LABORATORY APPLICATIONS

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ABSTRACT

Physics is one of the subjects that students find difficult to grasp due to the complexity of its abstract concepts and mathematical models. Consequently, students' interest and motivation regarding the course are often insufficient for effective learning. Overcoming these challenges requires an educational process that integrates theoretical and practical instruction; in other words, conducting experiments and practical work is crucial in physics education. However, laboratory work faces obstacles such as inadequate physical facilities in schools, equipment costs, safety risks, and time constraints. Given the strong connection students have with information technologies today, the impact of using virtual laboratories in physics classes on academic achievement, conceptual understanding, and attitudes toward the subject becomes more apparent. This study demonstrates how virtual laboratories enable students to safely and cost-effectively explore micro-level phenomena and conduct physics experiments that would otherwise be dangerous or impossible to perform in a school setting. Furthermore, the use of information technologies offers students an enjoyable learning environment. These virtual laboratory applications enhance problem-solving skills, allow for self-paced learning, and promote equal opportunity in education. The six experiment topics selected for this study address a recognized need for virtual laboratory experiments; making them accessible to students will help fulfill a significant requirement in this field. Ultimately, the virtual laboratory experiments featured in this study should be viewed not as a replacement for traditional laboratories, but as a complement that enhances the quality of physics education and fosters equal opportunity.

Keywords: Physics Teaching, Applied Education, Virtual Laboratory, Technology Integration in Education, Effective and Enjoyable Learning, Equality of Opportunity in Education

O-30

THE IMPACT OF DAMS ON CLIMATE CHANGE

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Large dams and reservoirs are traditionally championed as pillars of renewable energy and water security; however, emerging research highlights their complex, bidirectional relationship with global climate change. This paper synthesizes current empirical literature to evaluate the dual role of dams as both contributors to and victims of accelerating climatic shifts. First, we examine the biogeochemical mechanisms driving reservoir emissions, demonstrating that the anaerobic decomposition of flooded organic matter releases significant quantities of methane CH₄ and carbon dioxide CO₂, accounting for an estimated 1.3% of anthropogenic global greenhouse gas emissions. Second, we assess how climate-induced stressors threaten existing infrastructure. Altered hydrological cycles, prolonged droughts, and high-intensity precipitation events severely compromise hydropower efficiency and elevate the risks of spillway overtopping and catastrophic structural failure, particularly in aging dam fleets designed for historical stationary climates. Finally, we discuss the ecological ramifications of sediment trapping and altered microclimates. We conclude that future water management strategies must pivot away from traditional mega-dam paradigms, integrating rigorous emissions accounting and climate-resilient engineering to mitigate ecological degradation and safeguard downstream communities.

Keywords: Large Dams, Reservoir Emissions, Methane Footprint, Hydrological Volatility, Climate Resilience, Renewable Energy Paradox.

O-31

SIMULTANEOUS DETERMINATION OF ELEVEN MULTI-CLASS PESTICIDE RESIDUES IN CHERRIES BY LC-MS/MS: METHOD VALIDATION AND REAL SAMPLE ANALYSIS

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ABSTRACT

The widespread use of pesticides in fruit production necessitates the development of reliable analytical methods for residue monitoring to ensure food safety and regulatory compliance. In this study, a liquid chromatography–tandem mass spectrometry (LC–MS/MS) method was developed and validated for the simultaneous determination of eleven pesticides belonging to neonicotinoid, carbamate, organophosphate and triazole groups in cherry samples. Method validation was performed in accordance with SANTE document by evaluating linearity, sensitivity, accuracy, repeatability and reproducibility. The validated method exhibited satisfactory analytical performance with limits of quantification (LOQ) between 5.22 and 9.77 µg kg⁻¹. Recovery studies conducted at different spike levels demonstrated good accuracy, with repeatability recoveries ranging from 78.15–93.73% at 10 µg kg⁻¹ and 88.35–103.58% at 50 µg kg⁻¹. Reproducibility experiments yielded recoveries of 79.74–92.65% at 10 µg kg⁻¹ and 86.52–98.68% at 100 µg kg⁻¹. Relative standard deviation (%RSD) values for all analytes were <20%, indicating acceptable precision of the method. The validated method was subsequently applied to the analysis of ten commercial cherry samples collected from local markets. Among the ten cherry samples analyzed, all detected pesticide residues were below the established maximum residue limits (MRLs). Overall, the proposed LC–MS/MS method provides a sensitive, accurate and reliable approach for the determination of multiple pesticide residues in cherry matrices.

Keywords: pesticide, cherry, validation, LC–MS/MS

O-32

A COMPARATIVE ANALYSIS OF FEATURE ENGINEERING TECHNIQUES FOR MACHINE LEARNING-BASED HEART DISEASE PREDICTION

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ABSTRACT

Machine learning models are increasingly applied to support the early prediction of cardiovascular disease, yet most existing studies concentrate on model selection while giving comparatively little attention to how the underlying data is represented. Feature engineering, which shapes this representation, remains an under-examined stage of the modelling pipeline, and few studies compare its techniques within a common experimental framework. This study addresses that gap through a case study on the Cleveland Heart Disease dataset, applying and comparing several feature engineering strategies, namely dimensionality reduction (PCA), feature selection (RFE and SelectKBest), derived-feature generation, and class balancing through SMOTE, across four classifiers: Logistic Regression, Random Forest, Support Vector Machines, and Artificial Neural Networks. All techniques are evaluated within the same experimental setting using accuracy, F1-score, and ROC-AUC, and validated through k-fold cross-validation. The preliminary results indicate that dimensionality reduction through PCA tends to lower predictive performance, pointing to a loss of clinically relevant variance, whereas feature selection yields results broadly comparable to the baseline models. Generating new interaction- and ratio-based features appears to offer the most consistent improvement among the techniques considered, while class balancing through SMOTE does not provide a clear benefit given the relatively balanced class distribution of the dataset. Logistic Regression emerges as the most stable model across cross-validation folds. These preliminary findings suggest that carefully engineered features, rather than model complexity alone, can meaningfully improve the reliability of machine learning-based heart disease prediction; further experiments are being conducted to validate and extend these results before the final version of the study.

Keywords: Feature Engineering, Machine Learning, Heart Disease Prediction, Feature Selection

O-33

A COMPARATIVE ANALYSIS OF MACHINE LEARNING ALGORITHMS AND FEATURE ENGINEERING TECHNIQUES FOR ANXIETY LEVEL CLASSIFICATION: AN APPLICATION ON THE GAMINGSTUDY DATASET

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ABSTRACT

Anxiety among students has become a growing concern in education, as it is closely linked to academic performance and overall psychological well-being. Traditional assessment methods, such as surveys and clinical interviews, are informative but often time-consuming, subjective, and difficult to scale across large student populations. Data-driven approaches, particularly machine learning, offer a promising alternative for identifying anxiety patterns in a more systematic and scalable way. This study proposes a comparative framework for predicting student anxiety levels using several widely adopted machine learning algorithms, namely Logistic Regression, Support Vector Machine, Random Forest, Naive Bayes, and Artificial Neural Networks. The analysis is designed around the Student Anxiety Dataset, which combines Generalized Anxiety Disorder (GAD) scores with demographic, behavioral, and social-interaction indicators. Rather than focusing on algorithm comparison alone, the proposed framework places particular emphasis on the preprocessing pipeline that precedes model training, including missing-value handling, categorical encoding, feature scaling, dimensionality reduction through Principal Component Analysis, and resampling strategies such as SMOTE to mitigate class imbalance. Model performance is planned to be assessed using accuracy, precision, recall, F1-score, and ROC-AUC, with hyperparameter tuning carried out via grid and random search. By systematically relating preprocessing and feature engineering choices to the resulting performance of each algorithm, the study aims to clarify which methodological combinations are best suited to anxiety prediction tasks. The expected outcome is a practical, replicable methodology that can inform early-warning tools in educational settings and provide a reference point for future work at the intersection of machine learning and student psychological well-being.

Keywords: Student Anxiety, Machine Learning, Feature Engineering, Educational Data Mining, Classification Performance

O-34

CLONING, RECOMBINANT EXPRESSION, AND PURIFICATION OF HUMAN PAD4 IN *ESCHERICHIA COLI* BL21(DE3)

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ABSTRACT

Peptidylarginine deiminase 4 (PAD4) is a calcium-dependent enzyme involved in the conversion of protein-bound arginine residues into citrulline and has been associated with citrullination-related autoimmune processes, including rheumatoid arthritis. Recombinant production of human PAD4 provides an essential basis for further biochemical, immunological, and inhibitor-development studies targeting this enzyme. In this study, the human *PADI4* coding sequence was codon-optimized for bacterial expression and cloned into the pET-30a(+) expression vector, enabling the production of recombinant PAD4 with an N-terminal 6×His tag and enterokinase cleavage site. The recombinant pET-30a(+)-*PADI4* construct was transformed into chemically competent *Escherichia coli* BL21(DE3) cells, and kanamycin-resistant colonies were screened by colony PCR. Positive clones were further verified by sequence analysis. Recombinant PAD4 expression was induced with lactose, and the protein was purified from the soluble cell lysate by immobilized metal affinity chromatography. SDS-PAGE analysis demonstrated a prominent protein band at approximately 75 kDa in the elution fractions, consistent with the expected molecular size of recombinant PAD4. The purified protein was subsequently desalted into PBS, and the final concentration of recombinant PAD4 was determined as 0.8 mg/mL. These results demonstrate the successful cloning, bacterial expression, and purification of recombinant human PAD4, providing a purified antigen suitable for downstream functional and antibody-based studies.

Keywords: PAD4, *PADI4*, recombinant protein expression, *Escherichia coli* BL21(DE3), IMAC, rheumatoid arthritis

O-35

LIVING INTELLIGENCE (LI) IS LIVING ON INTELLIGENT SYSTEMS (ISs): CAN LI REALLY BE SOMETHING ALIVE WITH THEM?

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ABSTRACT

While *artificial intelligence* (AI) is the *intelligence* that is not *natural* / *biological* and artificial-by-design, *organic intelligence* (OI) represents the one that is *natural* and evolves over time. OI is found in *living organisms* / *entities* such as *animals*, *bacteria*, *cells*, *fungi*, *microorganisms*, and *plants*. To improve the *daily-life* of people and solve the *real-world* problems, *biotechnology* brings together *biology* and *technology*. For this purpose, it helps make better the *health*, *food*, *water*, and the *nature* of ours. This branch of science utilizes not only *living organisms* but also *biological processes and systems* to develop useful *products*, *technologies*, and *tools* for various applications. These applications are encountered in the fields such as *agriculture*, *environmental management*, *healthcare services*, *industry*, and *medicine*. In *biology* and *technology* living intelligence (LI), on the other hand, is a new phase. In this study, we address LI and how it is involved in *intelligent systems* (ISs), supported with some examples. Through the union of AI, *biotechnology*, and *sensors*, *self-organizing* and *dynamic* networks and systems are created. These autonomous (*self-governing*) systems can *continuously* perceive, *detect*, *learn*, *adapt*, and *evolve*, and therefore are ISs. Moreover, such tasks / operations are accomplished in *real-time*, without focusing on the data and datasets that are neither *current* nor *dynamic*. LI is an emerging *biological* and *technological* paradigm that sits between *living organisms* and *digital computers* / *machines*. This type of *intelligence* covers *cognitive* processes *consciously* and *intentionally* throughout the *biological* and *technological* systems. Additionally, these *adaptable* and *scalable* processes are studied at all *levels* and *scales* of the *life*, in terms of *biological cognition*. A system that is able to accomplish all the tasks handled by LI can be called an IS and may be *hybrid*. From this point, it can be said that LI is *living* on ISs or in other words is something *alive* with them. From the other side, AI turns into LI on ISs. As a result, we believe that this fact is *extremely* critical to take the actions needed for shaping the future in advance, especially in and for the current era as well as coming forms and versions of AI.

Keywords: Living Intelligence, Intelligent System, Artificial Intelligence, Organic Intelligence, Biotechnology, and Biological Cognition.

O-36

PREPARATION OF SILICA COATED ALUMINIUM NANOPARTICLES FOR COLORIMETRIC DETERMINATION OF GLUCOSE

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Developing highly sensitive, cost-effective, and robust colorimetric platforms for biomolecule detection is essential for advancing clinical diagnostics. While noble metal nanoparticles are widely used, aluminum nanoparticles (Al NPs) present an attractive, earth-abundant, and economical alternative for plasmonic biosensing. However, their structural instability and susceptibility to rapid ambient oxidation limit their practical application. To overcome these limitations, we report a highly stable and sensitive colorimetric biosensor for glucose determination utilizing core-shell silica-coated aluminum nanoparticles (Al@SiO₂ NPs). In this approach, Al NPs were synthesized via a controlled chemical reduction method and encapsulated with a uniform, protective silica shell using a modified Stöber process. This shell prevents core oxidation while providing a versatile framework for functionalization. The Al@SiO₂ surface was modified with (3-aminopropyl) triethoxysilane (APTES) to co-immobilize glucose oxidase (GOx) and horseradish peroxidase (HRP) via glutaraldehyde cross-linking. In the presence of glucose, the cascade enzymatic reaction generates hydrogen peroxide (H₂O₂), driving the HRP-catalyzed oxidation of the chromogenic substrate 3,3',5,5'-tetramethylbenzidine (TMB) and producing a distinct colorless-to-blue transition. The localized surface plasmon resonance (LSPR) properties of the Al@SiO₂ core significantly enhanced the local electromagnetic field, amplifying the optical signal of the oxidized TMB dye. Under optimized conditions, the absorbance intensity at 652 nm exhibited a wide linear relationship with glucose concentrations across a clinically relevant range, achieving a nanomolar limit of detection (LOD). Furthermore, the Al@SiO₂-GOx/HRP biosensor demonstrated excellent selectivity against common physiological interferences, such as ascorbic acid, uric acid, and fructose, alongside high reproducibility. This work highlights the potential of Al@SiO₂ nanoparticles as a powerful, low-cost platform for plasmonic enzymatic cascades, offering great promise for next-generation point-of-care diagnostics.

Keywords: Aluminum nanoparticles; Core-shell nanostructures; Localized surface plasmon resonance (LSPR); Colorimetric sensing; Glucose determination, Enzyme immobilization.

O-37

CYBERSECURITY EDUCATION FOR INDUSTRY 5.0: A HUMAN-CENTRIC APPROACH WITHIN THE EU CYBER ECOSYSTEM

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ABSTRACT

Cybersecurity has evolved far beyond its original perception as a purely technical domain. Today, it represents a critical foundation for economic stability, national security, and public trust in digital systems. The rapid digitalization of industries, public services, and everyday life has significantly expanded the cyber threat landscape, making cybersecurity a strategic priority at both national and global levels.

At the same time, the transition towards Industry 5.0 introduces a fundamentally new perspective on technological development. Unlike Industry 4.0, which focused on automation, efficiency, and digital integration, Industry 5.0 emphasizes human-centricity, sustainability, and resilience. This shift redefines technology as a tool that must serve human needs, support societal well-being, and ensure long-term system stability.

In this context, cybersecurity becomes not only a technical necessity but also a key component of human-centered digital ecosystems. Universities, as primary institutions for knowledge creation and skills development, play a decisive role in preparing professionals capable of addressing complex cybersecurity challenges within this new paradigm. The transition to Industry 5.0 significantly increases the complexity and scale of cybersecurity challenges. Modern digital environments are characterized by the integration of artificial intelligence, cloud computing, the Internet of Things (IoT), and cyber-physical systems, each introducing new vulnerabilities and attack vectors.

O-38

THE DIRAC EQUATION AS GEOMETRIC NECESSITY: A CLIFFORD-ALGEBRA REFORMULATION

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ABSTRACT

The Dirac equation is generally accepted as the correct relativistic wave equation for spin-1/2 particles; however, its standard derivation does not explain why it must take this specific form. It is a first-order equation built from four-by-four gamma matrices acting on a four-component spinor. This article isolates a central objective, which is to show that reformulating the Dirac equation in Clifford (geometric) algebra reveals relativistic quantum mechanics to be a geometric expression of spacetime structure, rather than a set of algebraic rules chosen because they happen to work. Using the spacetime algebra formalism, the gamma matrices are replaced by an orthonormal frame of basis vectors, and the four-component complex spinor is replaced by an even-grade multivector, a scalar plus a bivector.

Carrying out the derivation in this language shows that the anticommutation relations defining the Clifford algebra, the first-order structure of the wave equation, and the four-dimensionality of the spinor are not independent postulates but direct and forced consequences of the Minkowski metric signature. The matrix and geometric formulations are shown to be mathematically equivalent, reproducing identical predictions, which confirms that the geometric reformulation introduces no new physics, only a different, more transparent derivation of the same physics. The result reframes a well-established equation: the Dirac equation is not merely consistent with the geometry of spacetime; it is the only equation that is consistent with it.

Keywords: Geometric Algebra, Dirac Equation, Gamma Matrices, Spinor, Spacetime Geometry

BENCHMARKING AI MODELS FOR SYMBOLIC TURKISH MAKAM MUSIC GENERATION ON A SYMBOLIC TURKISH MAKAM MUSIC DATASET

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ABSTRACT

Recent advances in artificial intelligence have significantly advanced symbolic music generation, with most existing studies focusing on Western tonal music. In contrast, Turkish makam music has received comparatively limited attention despite its rich modal structure, microtonal characteristics, and complex melodic organization. These distinctive musical features present unique challenges for symbolic music generation and require dedicated benchmark studies to evaluate the capabilities of modern generative models.

This study presents a comparative benchmark of three representative artificial intelligence models for symbolic Turkish makam music generation using a large-scale symbolic Turkish makam music dataset. Three widely adopted sequence generation approaches representing different modeling paradigms are investigated: Markov Chain, Long Short-Term Memory (LSTM), and Transformer. To ensure a fair and reproducible comparison, all models are trained and evaluated using the same symbolic representations, preprocessing pipeline, and experimental protocol.

The generated musical sequences are assessed using both computational and musicological evaluation criteria. Quantitative analyses include pitch distribution similarity, interval statistics, melodic contour preservation, sequence diversity, and phrase coherence. Furthermore, makam-specific

musical characteristics, including modal consistency, melodic progression, and stylistic preservation, are examined to evaluate the authenticity and musical quality of the generated compositions. Computational efficiency and generation performance are also compared across the three approaches.

The proposed benchmark provides a systematic comparison of classical probabilistic and deep learning methods for symbolic Turkish makam music generation. The findings are expected to establish a reproducible evaluation framework for culturally informed music generation while providing practical insights into the suitability of different artificial intelligence models for preserving the musical characteristics of Turkish makam music.

Keywords: Turkish Makam Music, Symbolic Music Generation, Artificial Intelligence, Markov Chain, LSTM, Transformer, Music Information Retrieval, Computational Musicology.



FULL TEXTS

EFFECTS OF DATA SPLITTING STRATEGIES ON RECOMMENDER SYSTEM EVALUATION

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ABSTRACT

Offline evaluation is widely used to compare recommender systems, but its results can change with the selected data splitting strategy. Earlier studies showed that split choice, temporal leakage, random seeds, and sampling can change accuracy and model rankings. However, most studies examine a limited set of model families, focus mainly on accuracy, or study a single domain or recommendation task. They rarely compare traditional, deep learning, and graph-based methods in the same software environment while also considering dataset density and computational cost. This study addresses this research problem by evaluating nine algorithms with a ratio split, a user based stratified split, and 5-fold cross-validation. The experiments use the relatively dense MovieLens-100K dataset and a sparse Amazon-Toys subset. Accuracy is measured with normalized discounted cumulative gain at 10 (NDCG@10), Precision@10, Recall@10, and F1@10. Both training and test times are also reported. On MovieLens-100K, the Multi-Layer Perceptron with five-fold cross-validation gives the highest NDCG@10 value of 0.2153. On Amazon-Toys, Neural Graph Collaborative Filtering with the ratio split gives the highest NDCG@10 value of 0.0446. The findings show that the best split depends on the algorithm and dataset. 5-fold cross validation often improves ranking accuracy, especially on the sparse dataset, but the ratio split and stratified split also produce the best results for some algorithms. 5-fold cross validation also increases total runtime because each algorithm is trained and tested five times. Therefore, data splitting should be treated as a main part of recommender system evaluation rather than a minor implementation choice.

Keywords: Data splitting, recommender systems, offline evaluation, accuracy, computational cost

1. INTRODUCTION

Recommender systems help users find relevant items in large collections. Early systems mainly used neighborhood methods and matrix factorization. User-based k-nearest neighbors (UserKNN) and item-based k-nearest neighbors (ItemKNN) estimate preferences from similar users or items, while matrix factorization represents users and items in a shared latent space [1]. Later, deep learning methods such as Neural Collaborative Filtering and variational autoencoders were developed to learn more complex user-item relations [2,3]. Graph-based methods, including Neural Graph Collaborative Filtering (NGCF), model interactions as a user-item graph and pass information between connected users and items [4].

As recommendation models became more complex, concerns about evaluation quality also increased. Several studies showed that advanced neural models do not always outperform well-tuned traditional baselines [5,6]. Offline results depend not only on the algorithm but also on preprocessing, hyperparameters, candidate selection, evaluation metrics, and data splitting [7]. Data splitting is especially important because it decides which interactions are available for learning and which interactions are used for testing. A different split can change user and item coverage, interaction density, and the information available to the model. Random non-temporal splits may also place later interactions in the training data and earlier interactions in the test data. When timestamps are available, this may cause temporal leakage and produce results that do not represent a real future-recommendation setting [8].

A growing body of research has examined these problems from different viewpoints. Chou et al. studied time-based splitting and evaluation metrics for music recommendation [9]. Meng et al. compared three common splitting strategies across seven recommendation models and two datasets [10]. They showed that the selected strategy can change model rankings even when the dataset and metrics remain the same. Zhao et al. reviewed the main choices in offline top-ranked recommendation evaluation and showed that evaluation settings must be selected carefully [7]. Ji et al. focused on violations of the global timeline and showed that leaked future interactions can change both accuracy and model order [8]. Wegmeth et al. examined random seeds in hold-out splitting and found that a single seed can overestimate or underestimate performance; they also showed that cross-validation reduces this variation [11]. Sachdeva et al. studied dataset sampling and showed that sampling choices can also change algorithm performance and rankings [12].

Other studies have focused on narrower recommendation tasks or on tools for reproducible evaluation. Gusak et al. compared leave-one-out and global temporal protocols for sequential recommendation and showed that the split can affect model rankings and deployment decisions [13]. Turksoy and Turkmen compared random and temporal splits for click-through-rate (CTR) prediction [14]. Elliot provides a common framework for reproducible recommender-system experiments with several evaluation options [15]. More recently, SplitLight was introduced to inspect split validity, temporal leakage, cold users and items, and distribution changes [16]. These works confirm that splitting is an important part of evaluation. However, they mainly study temporal realism, sequential recommendation or CTR tasks, seed variation, dataset sampling, or split auditing. Even the broad study by Meng et al. [10] evaluates a different set of splitting rules and does not examine the exact combination considered here: a global random ratio split, a user-stratified split, and five-fold cross-validation. The combined effect of these three common non-temporal strategies on traditional, deep learning, and graph-based algorithms has also received limited attention, especially when dataset density and training and test costs are considered together.

This study addresses this research problem through a controlled benchmark in the Cornac framework. Nine algorithms are evaluated in three groups: traditional methods consisting of UserKNN, ItemKNN, Probabilistic Matrix Factorization (PMF), and Matrix Factorization (MF); deep learning methods consisting of Neural Matrix Factorization (NeuMF), Multi-Layer Perceptron (MLP), and

Variational Autoencoder for Collaborative Filtering (VAECF); and graph-based methods consisting of Graph Convolutional Matrix Completion (GCMC) and NGCF. Each algorithm is tested with the same three splitting strategies: ratio split (80/20), stratified split (80/20), and five-fold cross-validation. The experiments use the relatively dense MovieLens-100K dataset and a highly sparse Amazon-Toys subset. Unlike studies limited to one model family or one application area, this work compares three generations of recommenders under one implementation environment. Unlike studies that focus only on accuracy, it evaluates normalized discounted cumulative gain at 10 (NDCG@10), precision at 10 (Precision@10), recall at 10 (Recall@10), and F1-score at 10 (F1@10), together with training and test times. The aim is to identify how split choice changes the winning strategy for each algorithm, whether these patterns differ across model families and dataset densities, and how much computational cost is added by a more extensive evaluation protocol.

2. MATERIAL AND METHOD

2.1. Experimental Environment & Tools

All experiments were carried out with the open-source Cornac framework [17]. Cornac provides a common interface for recommendation algorithms, data splitting methods, and evaluation metrics. Using a common evaluation framework helps reduce methodological differences caused by separate implementations [18]. The experiments were run on a workstation with an Intel Xeon E5-2643 v2 CPU and 128 gigabytes of third-generation DDRAM. No graphics processing unit was used. The random seed was set to 42 for all data splitting strategies. The default Cornac parameters were used for all algorithms so that the models could be compared under a common and reproducible setup.

2.2. Datasets

Two datasets were selected to examine the effect of data density. MovieLens-100K is a widely used benchmark with 100,000 ratings from 943 users on 1,682 movies [19]. Its density is about 6.3047%. The second dataset is a subset of Amazon-Toys obtained through Cornac. Users with fewer than five ratings were removed. After this filtering step, the dataset contained 133,837 interactions from 15,529 users on 9,697 items, with a density of about 0.0889%. The Amazon review data are linked to the public dataset introduced by McAuley et al. [20]. The structural differences between the two datasets are summarized in Table 1.

Table 1. Statistical Characteristics of Dataset

Dataset Name	User Count	Item (Product) Count	Interaction (Vote) Count	Occupancy (Density) Rate
MovieLens-100K	943	1,682	100,000	6.3047%
Amazon-Toys (5-Core)	15,529	9,697	133,837	0.0889%

2.3. Data Splitting Strategies

Three splitting strategies were selected because they represent common but different offline evaluation settings. Ratio split provides a simple and low-cost hold-out evaluation. User-stratified split preserves the training-test proportion within each user and helps examine the effect of user-level balance. Five-fold cross-validation reduces dependence on one hold-out sample and provides a broader estimate by rotating the test data. Comparing these methods makes it possible to study the trade-off between simplicity, user-level control, evaluation stability, and computational cost.

Ratio Split (80/20): Representing the most fundamental partitioning method in machine learning, this strategy randomly allocates 80% of the global interactions to the training set and 20% to the test set. While computationally cheap, it is highly susceptible to random seed variance [11]. It may also create temporal leakage when interaction time is ignored [8].

User-Stratified Split (80/20): This method ensures that the 80/20 partition is strictly maintained on a per-user basis. It is crucial in recommender systems evaluation to avoid cold-start, guaranteeing that every user present in the test set has an adequate representation in the training set.

5-Fold Cross-Validation: The data were divided into five folds. Each fold was used once as the test set, while the other four folds were used for training. The reported accuracy values are the fold-level averages. The reported training and test times are accumulated across the five runs. Therefore, an increase close to five times is expected even when the cost of one run does not change. Cross-validation reduces dependence on one hold-out sample [21,22], but it is more expensive.

2.4. Recommendation Algorithms

To present a comprehensive benchmark, we meticulously selected nine algorithms representing the three primary generations of recommender systems: Traditional Machine Learning (focusing on linear relationships and latent spaces), Deep Learning (focusing on non-linear feature interactions), and Graph-based Paradigms (focusing on high-order structural connectivities). This covers a broad evolutionary spectrum of the field.

Traditional collaborative filtering-based approaches:

- UserKNN: A traditional memory-based collaborative filtering approach that generates recommendations by computing historical similarity scores among users [23].
- ItemKNN: A scalable neighborhood method that computes similarities between items rather than users to predict future preferences [24].

- PMF: A traditional latent factor model that extends standard factorization by incorporating probabilistic linear modeling for large, sparse datasets [25].
- MF: The foundational model that maps both users and items to a joint latent factor space to capture explicit and implicit interactions [1].

Deep learning-based approaches:

- NeuMF: A deep learning architecture that fuses generalized matrix factorization with a multi-layer perceptron to learn non-linear user-item interactions [2].
- MLP: A neural collaborative filtering model that uses multiple hidden layers to learn non-linear user-item interactions instead of relying on the conventional inner-product interaction function used in matrix factorization [2].
- VAE CF: A principled deep generative model that utilizes multinomial likelihoods to learn robust latent representations of user preferences [3].

Graph-based approaches

- GCMC: A graph neural network model that frames recommendation as a link prediction task using spatial graph convolutions [26]. Since default implementation of GCMC in Cornac requires a validation set a 70:10:20 data splitting is utilized for only GCMC.
- NGCF: A state-of-the-art graph architecture that explicitly models higher order connectivities by injecting collaborative signals directly into the embedding propagation process [4].

2.5. Evaluation Metrics

Ranking accuracy was evaluated with normalized discounted cumulative gain at 10 (NDCG@10), precision at 10 (Precision@10), recall at 10 (Recall@10), and F1-score at 10 (F1@10). Higher values indicate better top-10 recommendation quality. NDCG@10 also gives more weight to relevant items that appear near the top of the list. Training time and test time were measured in seconds. For five-fold cross-validation, these times are totals over all five folds.

3. RESULTS

The empirical evaluation was conducted to benchmark the nine selected algorithms across the three data splitting strategies (ratio split, stratified split, and 5-fold cross validation) and two environments (MovieLens-100K and Amazon-Toys).

3.1. Analysis on MovieLens-100K Dataset

Table 2 presents the accuracy results for the MovieLens-100K dataset. Among the traditional methods, UserKNN performs best with the ratio split. Its NDCG@10 is 0.0005, which is 25.0% higher than the second-best value obtained with 5-fold cross validation. Its F1@10 is also 0.0005, which is 66.7% higher than the 5-fold cross validation value. ItemKNN also performs best with the ratio split. Its NDCG@10 of 0.0264 is 1.9% higher than the stratified split value of 0.0259. Its F1@10 of 0.0181 is 1.7% higher than the stratified split value of 0.0178. PMF performs best with 5-fold cross validation. Its NDCG@10 of 0.0857 is 0.7% higher than the ratio split value of 0.0851, and its F1@10 of 0.0557 is 1.1% higher than the ratio split value of 0.0551. MF performs best with the stratified split. Its NDCG@10 of 0.0719 is 2.1% higher than the 5-fold cross validation value of 0.0704, and its F1@10 of 0.0493 is 8.6% higher than the 5-fold cross validation value of 0.0454. Therefore, the traditional methods do not have one common winning strategy on MovieLens-100K. However, the neighborhood-based methods perform better when the ratio split is used.

The deep learning-based methods also show different responses to the splitting strategies. NeuMF performs best with the stratified split. Its NDCG@10 of 0.2119 is 2.5% higher than the ratio split value of 0.2068, and its F1@10 of 0.1414 is 0.9% higher than the ratio split value of 0.1401. MLP performs best with 5-fold cross validation for both metrics. Its NDCG@10 increases from 0.2040 with the stratified split to 0.2153, corresponding to an improvement of 5.6%. Its F1@10 increases from 0.1365 to 0.1392, representing an improvement of 2.0%. VAE CF performs best with the ratio split. Its NDCG@10 of 0.2142 is 1.7% higher than the stratified split value of 0.2106, and its F1@10 of 0.1378 is 0.9% higher than the stratified split value of 0.1366. These results show that the best split for a deep learning-based model can change from one algorithm to another.

For the graph-based methods, GCMC performs best with 5-fold cross validation. Its NDCG@10 of 0.1287 is 4.6% higher than the ratio split value of 0.1230, and its F1@10 of 0.0783 is 2.4% higher than the ratio split value of 0.0765. NGCF performs best with the ratio split. Its NDCG@10 of 0.0984 is 0.5% higher than the 5-fold cross validation value of 0.0979, and its F1@10 of 0.0698 is 1.2% higher than the 5-fold cross validation value of 0.0690. Thus, the graph-based methods do not have a common winning strategy on MovieLens-100K.

Overall, the ratio split gives the best NDCG@10 and F1@10 results for four algorithms, 5-fold cross validation gives the best results for three algorithms, and the stratified split gives the best results for two algorithms. The highest NDCG@10 in Table 2 is obtained by MLP with 5-fold cross validation. These findings show that the selected split can change the apparent ranking of algorithms, even on a relatively dense dataset.

Table 2. Accuracy Results for MovieLens-100K

Model	Split Method	NDCG@10	Precision@10	Recall@10	F1@10
UserKNN	Ratio Split	0.0005	0.0005	0.0005	0.0005
	Stratified Split	0.0002	0.0003	0.0002	0.0002
	5-Fold Cross-Validation	0.0004	0.0003	0.0004	0.0003
ItemKNN	Ratio Split	0.0264	0.0264	0.0159	0.0181
	Stratified Split	0.0259	0.0256	0.0148	0.0178
	5-Fold Cross-Validation	0.0244	0.0242	0.0144	0.0167
PMF	Ratio Split	0.0851	0.0731	0.0612	0.0551
	Stratified Split	0.0693	0.0651	0.0497	0.0488
	5-Fold Cross-Validation	0.0857	0.0748	0.0584	0.0557
MF	Ratio Split	0.0663	0.0609	0.0423	0.0433
	Stratified Split	0.0719	0.0689	0.0470	0.0493
	5-Fold Cross-Validation	0.0704	0.0652	0.0432	0.0454
NeuMF	Ratio Split	0.2068	0.1567	0.1866	0.1401
	Stratified Split	0.2119	0.1574	0.1840	0.1414
	5-Fold Cross-Validation	0.2062	0.1538	0.1805	0.1361
MLP	Ratio Split	0.2022	0.1492	0.1635	0.1284
	Stratified Split	0.2040	0.1547	0.1760	0.1365
	5-Fold Cross-Validation	0.2153	0.1596	0.1846	0.1392
VAECF	Ratio Split	0.2142	0.1615	0.1779	0.1378
	Stratified Split	0.2106	0.1563	0.1777	0.1366
	5-Fold Cross-Validation	0.2080	0.1565	0.1755	0.1342
GCMC	Ratio Split	0.1230	0.1034	0.0811	0.0765
	Stratified Split	0.1169	0.0993	0.0733	0.0729
	5-Fold Cross-Validation	0.1287	0.1073	0.0796	0.0783
NGCF	Ratio Split	0.0984	0.0780	0.0857	0.0698
	Stratified Split	0.0956	0.0747	0.0870	0.0687
	5-Fold Cross-Validation	0.0979	0.0763	0.0883	0.0690

Table 3 reports the training and test time in seconds for all the algorithms across different data splitting strategies on MovieLens-100K. The ratio split and stratified split have similar costs for most algorithms. For example, NeuMF requires 231.27 seconds for training with the ratio split and 219.61 seconds with the stratified split. MLP requires 218.62 and 218.75 seconds, respectively. These differences are small compared with the additional cost of 5-fold cross validation. The traditional methods remain computationally efficient. Under 5-fold cross validation, their training times range from 0.12 to 12.44 seconds, while their test times range from 9.70 to 40.81 seconds. Compared with the ratio split, the training and test times are generally about four to five times higher.

For the deep learning-based methods, the increase in training time under 5-fold cross validation is also close to the repeated-run cost. NeuMF training time increases from 231.27 to 1165.76 seconds, while MLP training time increases from 218.62 to 1160.20 seconds. VAECF is much faster to train than NeuMF and MLP, increasing from 7.89 to 48.50 seconds, although its test time is longer than those of NeuMF and MLP.

The graph-based methods have the highest absolute training costs, mainly because of NGCF. Its training time increases from 7273.72 seconds with the ratio split to 37658.44 seconds with 5-fold cross validation, corresponding to a 5.18-fold increase. GCMC increases from 77.89 to 335.11 seconds, corresponding to a 4.30-fold increase. These results show that 5-fold cross validation mainly adds the expected repeated-run cost. Because 5-fold cross validation trains and tests each algorithm five separate times, once for each fold, its total runtime is expected to be nearly five times higher than that of a single ratio or stratified split.

Table 3. Time Analysis for MovieLens-100K

Model	Split Method	Train Time (s)	Test Time (s)
UserKNN	Ratio Split	0.16	6.94
	Stratified Split	0.11	7.22
	5-Fold Cross-Validation	0.62	37.67
ItemKNN	Ratio Split	0.25	7.70
	Stratified Split	0.25	7.97
	5-Fold Cross-Validation	1.08	40.81
PMF	Ratio Split	2.56	1.77
	Stratified Split	2.55	1.80
	5-Fold Cross-Validation	12.44	9.70
MF	Ratio Split	0.03	2.81
	Stratified Split	0.02	2.86
	5-Fold Cross-Validation	0.12	15.22
NeuMF	Ratio Split	231.27	13.71
	Stratified Split	219.61	13.88
	5-Fold Cross-Validation	1165.76	70.98
MLP	Ratio Split	218.62	13.12
	Stratified Split	218.75	12.69
	5-Fold Cross-Validation	1160.20	64.59
VAECF	Ratio Split	7.89	16.12
	Stratified Split	7.81	16.53
	5-Fold Cross-Validation	48.50	97.32
GCMC	Ratio Split	77.89	21.19
	Stratified Split	62.31	20.58
	5-Fold Cross-Validation	335.11	102.73
NGCF	Ratio Split	7273.72	1.93
	Stratified Split	7200.61	1.95
	5-Fold Cross-Validation	37658.44	10.58

3.2. Analysis on Amazon-Toys Dataset

Table 4 shows the accuracy results for the Amazon-Toys dataset. Among the traditional methods, UserKNN performs best with 5-fold cross validation. Its NDCG@10 of 0.0025 is 4.2% higher than the ratio split value of 0.0024, and its F1@10 of 0.0015 is 15.4% higher than the ratio split value of 0.0013. ItemKNN performs best with the stratified split. Its NDCG@10 of 0.0104 is 4.0% higher than the 5-fold cross validation value of 0.0100, and its F1@10 of 0.0052 is 2.0% higher than the 5-fold cross validation value of 0.0051. PMF performs best with 5-fold cross validation. Its NDCG@10 of 0.0079 is 33.9% higher than the ratio split value of 0.0059, and its F1@10 of 0.0039 is 18.2% higher than the ratio split value of 0.0033. MF obtains the highest NDCG@10 with 5-fold cross validation. Its NDCG@10 of 0.0008 is 14.3% higher than the ratio split value of 0.0007. However, its F1@10 is 0.0004 for both the ratio split and 5-fold cross validation according to the rounded table values. Therefore, 5-fold cross validation is the most common winning strategy for the traditional methods on Amazon-Toys, but MF shows a tie in F1@10 when four-decimal values are considered.

For the deep learning-based methods, 5-fold cross validation is the winning strategy for NeuMF and MLP, while the ratio split is the winning strategy for VAECF. NeuMF reaches an NDCG@10 value of 0.0184, which is 7.0% higher than the ratio split value of 0.0172. Its F1@10 of 0.0086 is 2.4% higher than the ratio split value of 0.0084. MLP also performs best with 5-fold cross validation. Its NDCG@10 of 0.0112 is 10.9% higher than the stratified split value of 0.0101, and its F1@10 of 0.0056 is 14.3% higher than the stratified split value of 0.0049. VAECF performs best with the ratio split. Its NDCG@10 of 0.0335 is 3.4% higher than the stratified split value of 0.0324, and its F1@10 of 0.0156 is 4.0% higher than the 5-fold cross validation value of 0.0150. These findings show that even in the same deep learning-based group, the effect of the split depends on the algorithm.

For the graph-based methods, GCMC performs best with 5-fold cross validation. Its NDCG@10 of 0.0022 is 22.2% higher than the ratio split value of 0.0018, and its F1@10 of 0.0010 is 11.1% higher than the ratio split value of 0.0009. NGCF performs best with the ratio split. Its NDCG@10 of 0.0446 is 1.4% higher than the 5-fold cross validation value of 0.0440, and its F1@10 of 0.0208 is 1.5% higher than the 5-fold cross validation value of 0.0205. NGCF with the ratio split also provides the highest overall NDCG@10 and F1@10 values in Table 4.

Overall, 5-fold cross validation gives the best NDCG@10 result for six of the nine algorithms on Amazon-Toys. For F1@10, it gives the best result for five algorithms and ties with the ratio split for MF according to the four-decimal table values. However, the ratio split is best for VAECF and NGCF, and the stratified split is best for ItemKNN. This shows that 5-fold cross validation is often effective on the sparse dataset, but it is not universally superior. The best splitting strategy still depends on the algorithm and the selected metric.

Table 4. Accuracy Results for Amazon-Toys

Model	Split Method	NDCG@10	Precision@10	Recall@10	F1@10
UserKNN	Ratio Split	0.0024	0.0008	0.0044	0.0013
	Stratified Split	0.0020	0.0007	0.0043	0.0012
	5-Fold Cross-Validation	0.0025	0.0009	0.0050	0.0015
ItemKNN	Ratio Split	0.0095	0.0030	0.0159	0.0048
	Stratified Split	0.0104	0.0032	0.0176	0.0052
	5-Fold Cross-Validation	0.0100	0.0032	0.0171	0.0051
PMF	Ratio Split	0.0059	0.0020	0.0117	0.0033
	Stratified Split	0.0033	0.0010	0.0063	0.0017
	5-Fold Cross-Validation	0.0079	0.0024	0.0139	0.0039
MF	Ratio Split	0.0007	0.0002	0.0013	0.0004
	Stratified Split	0.0006	0.0002	0.0009	0.0003
	5-Fold Cross-Validation	0.0008	0.0003	0.0015	0.0004
NeuMF	Ratio Split	0.0172	0.0054	0.0273	0.0084
	Stratified Split	0.0169	0.0049	0.0263	0.0078
	5-Fold Cross-Validation	0.0184	0.0054	0.0288	0.0086
MLP	Ratio Split	0.0052	0.0020	0.0099	0.0031
	Stratified Split	0.0101	0.0031	0.0173	0.0049
	5-Fold Cross-Validation	0.0112	0.0035	0.0186	0.0056
VAECF	Ratio Split	0.0335	0.0099	0.0529	0.0156
	Stratified Split	0.0324	0.0088	0.0503	0.0143
	5-Fold Cross-Validation	0.0316	0.0095	0.0494	0.0150
GCMC	Ratio Split	0.0018	0.0005	0.0030	0.0009
	Stratified Split	0.0016	0.0005	0.0029	0.0008
	5-Fold Cross-Validation	0.0022	0.0006	0.0037	0.0010
NGCF	Ratio Split	0.0446	0.0129	0.0717	0.0208
	Stratified Split	0.0436	0.0119	0.0695	0.0196
	5-Fold Cross-Validation	0.0440	0.0127	0.0703	0.0205

Table 5 shows that data sparsity changes where the computational cost occurs in the Amazon-Toys dataset. UserKNN and ItemKNN require short training times, but their test stages are much more expensive. Under the ratio split, their test times are 1453.83 and 1453.65 seconds, respectively. Under the stratified split, these values increase to 2070.62 and 1767.87 seconds. These changes correspond to increases of 42.43% for UserKNN and 21.62% for ItemKNN. Under 5-fold cross validation, their total test times reach 15509.85 and 13662.65 seconds. These values are 10.67 and 9.40 times higher than the ratio split test times, respectively. This indicates that neighborhood search and candidate evaluation create the main computational cost for KNN-based methods on the large and sparse Amazon-Toys dataset. PMF and MF have low training costs, but their test times also increase under the different splitting strategies. The PMF test time increases from 24.96 seconds with the ratio split to 31.21 seconds with the stratified split and 132.95 seconds with 5-fold cross validation. Similarly, the MF test time increases from 38.65 to 47.34 and 205.99 seconds.

For the deep learning-based methods, the stratified split slightly reduces training time but increases test time. The NeuMF training time decreases from 341.79 seconds with the ratio split to 325.48 seconds with the stratified split, while its test time increases from 63.83 to 80.22 seconds. These changes correspond to a 4.77% decrease in training time and a 25.68% increase in test time. MLP shows a similar pattern. Its training time decreases from 336.91 to 319.81 seconds, while its test time increases from 60.80 to 76.30 seconds. These changes correspond to a 5.08% decrease in training time and a 25.49% increase in test time. The VAECF training time decreases from 453.71 to 447.23 seconds, while its test time increases from 66.28 to 81.14 seconds. These changes correspond to a 1.43% decrease in training time and a 22.42% increase in test time. Under 5-fold cross validation, both training and test times increase because each model is trained and evaluated across five folds.

The graph-based methods show different computational patterns. GCMC requires about 32.00 seconds for training under both the ratio and stratified splits, but its test time is much higher, increasing from 363.09 to 456.76 seconds. This corresponds to a 25.80% increase in test time. In contrast, NGCF has a relatively short test stage but a very long training stage. Its training time is 12199.83 seconds with the ratio split and 62763.97 seconds with 5-fold cross validation. The stratified split reduces its training time by 5.90%, from 12199.83 to 11479.51 seconds, but increases its test time by 27.15%, from 25.78 to 32.78 seconds. Overall, 5-fold cross validation has the highest total runtime because every algorithm is trained and tested once for each of the five folds.

Table 5. Time Analysis for Amazon-Toys

Model	Split Method	Train Time (s)	Test Time (s)
UserKNN	Ratio Split	4.66	1453.83
	Stratified Split	4.62	2070.62
	5-Fold Cross-Validation	23.72	15509.85
ItemKNN	Ratio Split	2.30	1453.65
	Stratified Split	2.27	1767.87
	5-Fold Cross-Validation	11.70	13662.65
PMF	Ratio Split	4.47	24.96
	Stratified Split	4.06	31.21
	5-Fold Cross-Validation	21.16	132.95
MF	Ratio Split	0.05	38.65
	Stratified Split	0.03	47.34
	5-Fold Cross-Validation	0.17	205.99
NeuMF	Ratio Split	341.79	63.83
	Stratified Split	325.48	80.22
	5-Fold Cross-Validation	1823.20	333.79
MLP	Ratio Split	336.91	60.80
	Stratified Split	319.81	76.30
	5-Fold Cross-Validation	1796.42	315.33
VAECF	Ratio Split	453.71	66.28
	Stratified Split	447.23	81.14
	5-Fold Cross-Validation	2761.52	393.70
GCMC	Ratio Split	31.64	363.09
	Stratified Split	31.17	456.76
	5-Fold Cross-Validation	160.91	1806.12
NGCF	Ratio Split	12199.83	25.78
	Stratified Split	11479.51	32.78
	5-Fold Cross-Validation	62763.97	138.62

4. CONCLUSION

This study analyzes how ratio splitting, stratified splitting, and 5-fold cross validation affect the offline evaluation of recommender systems. Nine algorithms from traditional, deep learning, and graph-based groups were tested on the relatively dense MovieLens-100K dataset and the sparser Amazon-Toys dataset.

The results show that the selected splitting strategy can change accuracy values and model rankings. No single strategy provides the best result for every algorithm and dataset. On MovieLens-100K, the ratio split gives the best NDCG@10 and F1@10 results for four algorithms, 5-fold cross validation for three algorithms, and the stratified split for two algorithms. On Amazon-Toys, 5-fold cross validation gives the best NDCG@10 and F1@10 results for six algorithms, while the ratio split and stratified split are still the best options for some algorithms. These results show that dataset density and algorithm type both affect the impact of the split strategy.

The splitting strategy also has a clear effect on computational cost. Ratio and stratified splits usually require similar training times, while 5-fold cross validation generally requires much more total time because each algorithm is trained and tested once for every fold. This additional cost becomes important for algorithms that already require long training or test times. Therefore, accuracy and runtime should be considered together when selecting an evaluation protocol.

This study has several limitations. Only two datasets and one software framework were used. The experiments used a single random seed and the default Cornac parameters, without model-specific hyperparameter tuning. In addition, all evaluated strategies were non-temporal. Future studies should use several random seeds and include temporal splitting strategies. They should also evaluate more datasets with different sizes, densities, and domains.

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F-2

MACHINE LEARNING PREDICTION OF BAND GAPS IN ABX_3 PEROVSKITES USING OPEN MATERIALS DATABASES AND COMPOSITION-BASED FEATURESMuhammet ARUCU^{1,*}, Ahmet AKKAYA¹¹Department of Computer Technologies, Bandırma Onyedi Eylül University, Gönen, Türkiye

ABSTRACT

Accurate knowledge of the electronic band gap is essential for the rational design of semiconductors used in photovoltaic and optoelectronic devices; however, first-principles calculations based on density functional theory (DFT) are computationally expensive when large chemical spaces must be screened. In this study, a machine learning framework that predicts the band gaps of ABX_3 perovskite compounds directly from their chemical composition is presented, without performing any new electronic structure calculations. A dataset of 1798 unique perovskite-type compositions (942 semiconductors/insulators and 856 metals), together with their DFT-computed band gaps, is retrieved from the open-access Materials Project database, and only the thermodynamic ground-state polymorph of each composition is retained in order to eliminate duplicate-composition noise and data leakage. For each compound, 148 composition-based descriptors, including elemental electronegativity, covalent radii, valence electron statistics, and melting temperatures, are generated using the matminer featurization library. Linear (Ridge) and ensemble-based (Random Forest and Gradient Boosting) regression models are trained and compared using five-fold cross-validation. The hyperparameter-optimized Gradient Boosting model achieves a mean absolute error of 0.56 eV and a coefficient of determination of 0.74, and permutation importance analysis reveals that the fraction of d valence electrons is the dominant descriptor, consistent with the role of transition-metal d states in defining the band edges of perovskites. The results demonstrate that open-database-driven machine learning is a practical and computationally inexpensive screening tool for the discovery of candidate perovskite absorbers in energy applications. All calculations are implemented in Python using open-source libraries.

Keywords: Machine learning, band gap prediction, perovskites, Materials Project, computational physics

1. INTRODUCTION

Perovskite compounds with the general formula ABX_3 constitute one of the most versatile families of functional materials, spanning oxide ferroelectrics, photocatalysts, and, most prominently in the last decade, halide perovskite solar absorbers whose power conversion efficiencies have risen at an unprecedented rate [1, 2]. For nearly all of these applications the electronic band gap is the central design parameter: it determines the optical absorption onset of a photovoltaic absorber, the emission wavelength of a light-emitting device, and the transparency window of a dielectric. The ability to estimate the band gap of a candidate composition quickly and cheaply is therefore of direct practical value for materials screening in energy applications.

First-principles calculations based on density functional theory (DFT) are the standard tool for computing band structures, and large open databases such as the Materials Project now provide DFT-computed properties for hundreds of thousands of inorganic compounds [3]. Nevertheless, a full DFT calculation for every hypothetical composition remains computationally demanding, and semilocal exchange-correlation functionals of the generalized gradient approximation (GGA) type are known to systematically underestimate band gaps relative to experiment [8]. These observations motivate surrogate models that learn the mapping from chemical composition to the DFT band gap and can subsequently evaluate thousands of candidate compositions in seconds.

Machine learning (ML) approaches built on composition-based descriptors have proven remarkably successful for this task. Ward et al. introduced the general-purpose Magpie descriptor set, in which statistics of elemental properties are used as features for arbitrary compositions [4], and the matminer library provides an open-source implementation of this and many related featurizers [5]. Zhuo et al. demonstrated accurate band gap prediction for inorganic solids from composition alone [6], and Pilia et al. applied similar ideas specifically to perovskite chemistries [9]. Ensemble tree methods such as Random Forests [10] and Gradient Boosting [11] are typically the best-performing algorithms in this setting. However, the metrics reported in composition-based studies are rarely corrected for duplicate polymorph compositions in the underlying databases, an evaluation issue that is addressed explicitly in the present work.

In this work, an end-to-end, fully open-source ML pipeline for band gap prediction in the ABX_3 perovskite family is presented. The contributions are threefold. First, a curated dataset of 1798 unique perovskite-type compositions is constructed from the Materials Project [3, 12], in which only the thermodynamic ground-state polymorph of each composition is retained; it is shown that this deduplication step is essential for honest model evaluation, because identical compositions with different polymorph band gaps otherwise leak between training and test sets. Second, three regression algorithms are systematically compared under five-fold cross-validation with hyperparameter optimization. Third, the trained models are interpreted through permutation importance and validated against well-known perovskites with experimentally measured gaps. The complete workflow runs in a standard Python environment [7] without any commercial software or new DFT calculations.

2. MATERIALS AND METHODS

2.1. Dataset construction. All entries matching the anonymous formula ABC_3 (three elements in 1:1:3 stoichiometry) were retrieved from the Materials Project database through its application programming interface [3] (database accessed in August 2026), together with their PBE-GGA band gaps and thermodynamic stability data. Entries with an energy above the convex hull larger than 0.10 eV/atom were discarded. Because composition-based features cannot distinguish polymorphs, all remaining entries were grouped by

composition and only the lowest-energy (ground-state) polymorph of each formula was retained. The final dataset contains 1798 unique compositions, of which 942 are semiconductors or insulators ($E_g > 0$) and 856 are metals ($E_g = 0$). Because the anonymous-formula query selects on stoichiometry rather than on crystal structure, the dataset also contains non-perovskite ABX_3 structure types such as ilmenite-type oxides and carbonates; structure matching against the cubic perovskite aristotype shows that 828 of the 1798 compositions (46%) crystallize in a perovskite-type framework. The dataset is therefore best described as ABX_3 -type compositions, and all results below refer to this broader chemical family. Figure 1(a) shows the distribution of the nonzero band gaps, which extends up to approximately 8 eV with a median of 2.14 eV, and Figure 1(b) maps the occurrence of each chemical element in the dataset onto the periodic table. Oxygen is the dominant anion (743 compounds), while the halides F, Cl, Br, and I are also well represented, so that the dataset covers both oxide and halide perovskite chemistries.

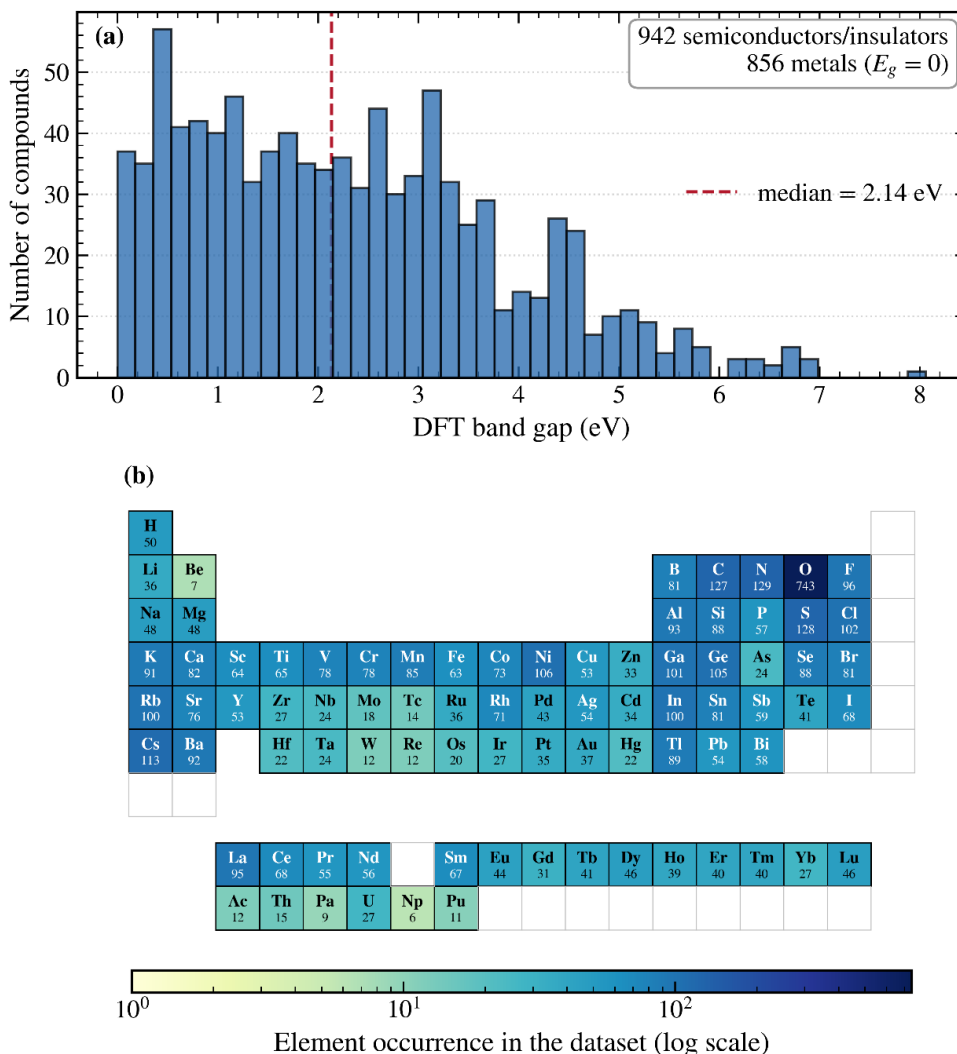


Figure 1. Overview of the ABX_3 dataset: (a) distribution of the DFT band gaps of the 942 semiconducting compositions (dashed line: median, 2.14 eV); (b) periodic-table heatmap of element occurrence (logarithmic color scale).

2.2. Feature generation. Each composition was converted into a fixed-length feature vector using the matminer library [5]. Four complementary featurizers were combined: (i) the Magpie elemental-property statistics (132 descriptors, including means, ranges, and deviations of electronegativity, covalent radius, valence electron counts, ionization-related quantities, and melting temperature) [4]; (ii) valence orbital occupation attributes (average and fractional s, p, d, and f valence electrons); (iii) stoichiometric p-norms; and (iv) the estimated band center derived from elemental electronegativities. In total, 148 composition-based descriptors were generated per compound; no structural information was used.

2.3. Models and evaluation protocol. Three regression algorithms implemented in scikit-learn [7] were compared: Ridge regression as a regularized linear baseline, Random Forest [10], and histogram-based Gradient Boosting [11]. The hyperparameters of the two ensemble models were optimized by randomized search with three-fold cross-validation. All random operations used a fixed seed, and the optimized hyperparameter values are documented in the openly shared analysis notebook. In addition, a nested cross-validation scheme, in which the randomized search is repeated inside each outer training fold, was employed to verify that hyperparameter selection does not leak information into the reported metrics. Model performance was then assessed by five-fold cross-validation on the 942 semiconducting compounds, using the mean absolute error (MAE), the root mean square error (RMSE), and the coefficient of determination (R^2) as metrics. For visualization and interpretation, an additional 80/20 train/test split was used; feature relevance was quantified by permutation importance on the held-out test set, and the data-size dependence of the error was characterized by a learning curve. Finally, a Random Forest classifier was trained on the full dataset (metals and non-metals) to address the auxiliary metal versus non-metal classification task.

3. RESULTS AND DISCUSSION

3.1. Regression performance. Table 1 summarizes the five-fold cross-validation results of the three models, and Figure 2 shows the same comparison graphically. Both ensemble methods clearly outperform the linear baseline: the MAE decreases from 0.83 eV for Ridge regression to 0.56 eV for the tuned ensembles, and R^2 increases from 0.53 to 0.74. Random Forest and Gradient Boosting perform comparably (0.564 ± 0.032 eV versus 0.561 ± 0.030 eV), indicating that the residual error is dominated by the information content of the composition-only representation rather than by the choice of ensemble algorithm. The nested cross-validation described in Section 2.3 yields an MAE of 0.561 ± 0.032 eV for the Gradient Boosting model, confirming that the selection bias introduced by the hyperparameter search is negligible. The obtained accuracy is also consistent with the range reported for composition-only models in the Matbench benchmark suite [17].

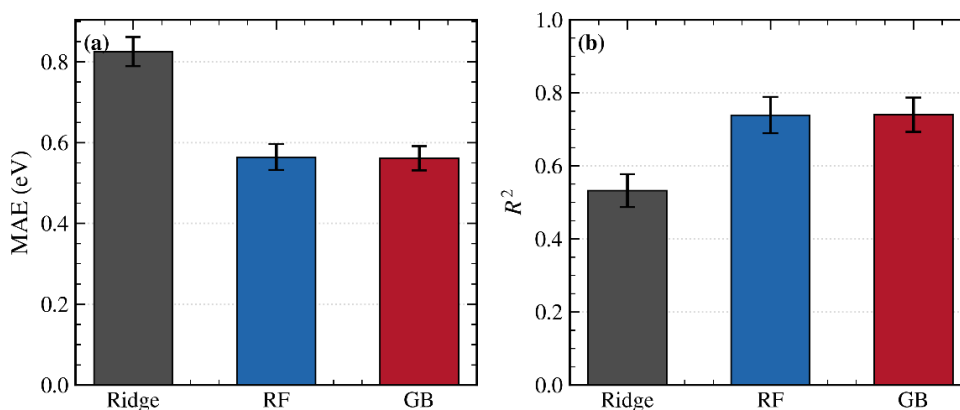


Figure 2. Five-fold cross-validated (a) MAE and (b) R^2 of the three regression models. Error bars denote one standard deviation over the folds.

Table 1. Five-fold cross-validation performance of the three regression models

Model	MAE (eV)	RMSE (eV)	R^2
Ridge	0.825 ± 0.036	1.054 ± 0.059	0.532 ± 0.045
Random Forest	0.564 ± 0.032	0.784 ± 0.072	0.739 ± 0.050
Gradient Boosting	0.561 ± 0.030	0.784 ± 0.073	0.740 ± 0.047

Figure 3 presents the parity plot of the tuned Gradient Boosting model on the held-out test set, where an MAE of 0.57 eV, an RMSE of 0.76 eV, and $R^2 = 0.77$ are obtained; the slightly higher single-split values relative to the cross-validated averages in Table 1 reflect split-to-split variability and should not be over-interpreted. The point density concentrates along the identity line over the whole 0-8 eV range, showing that the model does not simply regress toward the mean of the distribution. The largest scatter occurs for narrow-gap compounds ($E_g < 1$ eV), a known difficulty of composition-only models near the metal/semiconductor boundary [6]. The corresponding error distribution (Figure 4) is single-peaked and nearly centered at zero (mean +0.08 eV, standard deviation 0.76 eV), confirming the absence of a strong systematic bias.

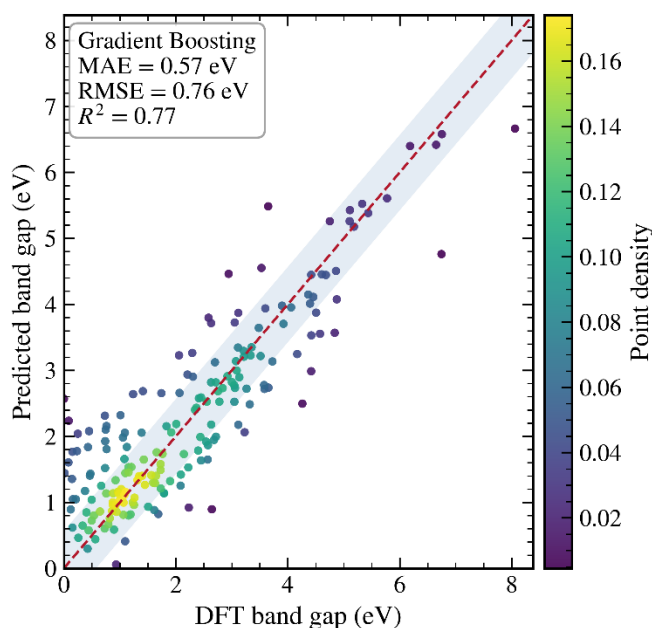


Figure 3. Parity plot of the tuned Gradient Boosting model on the held-out test set. Points are colored by local density; the shaded band indicates $\pm$ MAE around the identity line.

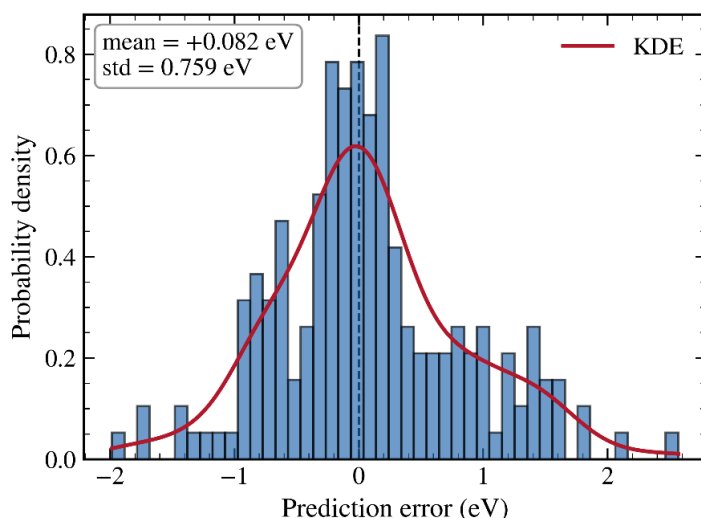


Figure 4. Distribution of the prediction errors on the test set together with a kernel density estimate.

3.2. Effect of dataset deduplication. It is worth emphasizing the role of the ground-state deduplication step introduced in Section 2.1. When all polymorphs are retained, identical feature vectors with different target values appear simultaneously in the training and test folds; in a controlled ablation using identical descriptors and identical tuned hyperparameters, retaining all polymorphs lowers the apparent cross-validated MAE from 0.561 eV to 0.489 ± 0.015 eV, an artificial improvement that silently degrades the honesty of the evaluation. Reporting metrics on deduplicated, composition-unique data is therefore recommended for all composition-based band gap studies.

3.3. Feature importance. Figure 5 shows the twelve most relevant descriptors according to permutation importance on the test set. The fraction of d valence electrons is by far the dominant feature, followed by the mode of the elemental melting temperatures and by valence-shell occupation statistics. This ranking has a clear physical interpretation: in oxide and halide perovskites the conduction band minimum is typically derived from the transition-metal d states of the B-site cation, so a descriptor counting d electrons directly encodes the character of the band edges. The elemental melting temperature acts as a proxy for bond strength and cohesive energy, which correlate with band gap width, while the average deviation of the electronegativity measures the ionicity of the A-X and B-X bonds, consistent with the classical trend that more ionic compounds exhibit wider gaps. It should nevertheless be kept in mind that permutation importance can concentrate the credit of a group of mutually correlated descriptors onto a single representative; the ranking should therefore be read as indicative rather than causal.

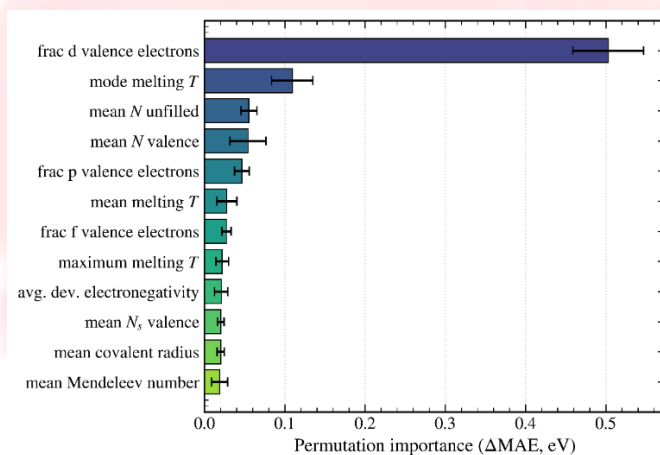


Figure 5. Twelve most relevant descriptors according to permutation importance (Δ MAE) on the test set. Error bars denote the standard deviation over 10 shuffles.

3.4. Learning behavior and classification. The learning curve of the Gradient Boosting model (Figure 6) shows that the cross-validated MAE decreases monotonically with the number of training compounds and has not yet saturated at the full dataset size, while the training error remains low. The model is therefore data-limited rather than capacity-limited, and its accuracy is expected to improve further as open databases grow. For the auxiliary metal versus non-metal task, the Random Forest classifier reaches a five-fold cross-validated accuracy of 0.879 ± 0.013 and an F1 score of 0.888 ± 0.010 (non-metal class), so that the full pipeline can first screen out metallic candidates before the regression stage is applied. The misclassified compounds concentrate near the metal/semiconductor boundary, consistent with the enhanced scatter observed for narrow-gap compounds in Figure 3.

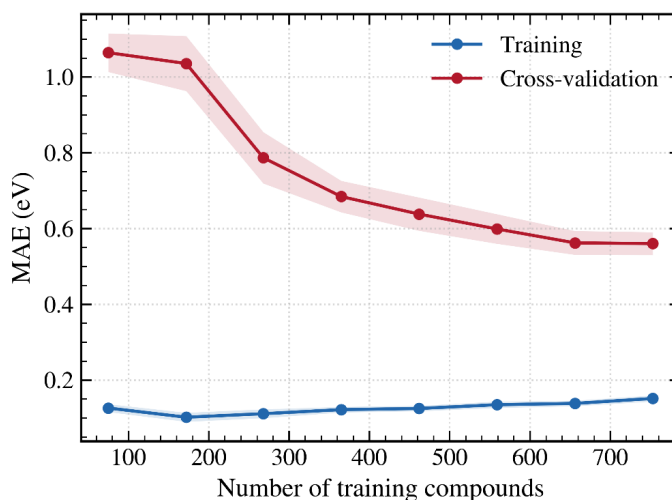


Figure 6. Learning curve of the Gradient Boosting model: training and cross-validated MAE as a function of the number of training compounds. Shaded areas denote one standard deviation.

3.5. Validation on well-known perovskites. Table 2 compares the ML predictions with the DFT-GGA values and with experimental band gaps for eight prototypical perovskites. The ML model tracks its DFT training labels closely (e.g., LaAlO_3 : 3.78 eV predicted versus 3.71 eV DFT), which is the expected and correct behavior of a surrogate model. At the same time, the table makes the systematic GGA underestimation explicit: for the oxide perovskites the experimental gaps exceed the GGA values by 1-2 eV (e.g., SrTiO_3 : 3.25 eV experimental versus 1.86 eV GGA), whereas for the halide perovskites CsPbX_3 the deviation is smaller and partly masked by the neglect of spin-orbit coupling in the reference calculations [16]. Predictions of the present model should therefore be interpreted as GGA-level estimates, and a constant or learned correction must be applied when experimental-scale gaps are required. A further caveat applies to CsPbI_3 : the experimental value of 1.73 eV refers to the black perovskite phase [14], whereas the ground-state polymorph retained by the deduplication rule is the non-perovskite yellow δ phase, so that the experimental and computed entries in this row correspond to different polymorphs.

Table 2. ML predictions compared with DFT-GGA and experimental band gaps [13-15] for prototypical perovskites

Formula	Exp. gap (eV)	DFT-GGA gap (eV)	ML prediction (eV)
BaTiO_3	3.20	2.29	3.26
CaTiO_3	3.50	2.31	2.90
CsPbBr_3	2.30	2.88	2.68
CsPbI_3	1.73	2.52	2.46
KNbO_3	3.30	2.31	2.34
LaAlO_3	5.60	3.71	3.78
NaTaO_3	4.00	2.59	2.77
SrTiO_3	3.25	1.86	2.31

The main limitation of the present approach is intrinsic to the composition-only representation: polymorphism, strain, and defect effects, as well as the structure-type heterogeneity of the dataset discussed in Section 2.1, are invisible to the model, and the accuracy ceiling observed here (about 0.55 eV MAE) reflects this information loss. Structure-aware models such as graph neural networks [18], and training labels computed with hybrid functionals or many-body methods, are natural extensions of this work.

4. CONCLUSION

A fully open-source machine learning pipeline for predicting the band gaps of ABX_3 perovskites directly from chemical composition has been presented. Using 1798 unique ground-state compositions from the Materials Project and 148 matminer descriptors, a hyperparameter-optimized Gradient Boosting model achieves a cross-validated MAE of 0.56 eV and $R^2 = 0.74$, with the fraction of d valence electrons identified as the physically dominant descriptor. The ground-state deduplication of the dataset was shown to be essential for honest evaluation, and the comparison with experimental gaps quantifies the systematic GGA underestimation that any database-trained surrogate inherits. The learning curve indicates that the accuracy will continue to improve as open materials databases grow. The entire workflow runs in minutes on free cloud hardware and can be applied as an immediate pre-screening filter in the computational discovery of perovskite absorbers for energy applications.

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F-3

TRANSFER MATRIX ANALYSIS OF ONE-DIMENSIONAL PHOTONIC CRYSTALS: DESIGN OF BRAGG REFLECTORS AND DEFECT-MODE OPTICAL FILTERS

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ABSTRACT

One-dimensional photonic crystals, consisting of periodically alternating dielectric layers, exhibit photonic band gaps in which the propagation of light is forbidden, and they form the basis of high-reflectivity mirrors, optical filters, and sensing platforms. In this work, the optical response of one-dimensional photonic crystal structures is investigated numerically by means of the transfer matrix method (TMM) implemented entirely in Python using open-source libraries. The implementation is verified against four independent analytic results, including the exact single-film reflectance formula, with agreement at machine precision (deviations below 10^{-16}). Quarter-wave $\text{SiO}_2/\text{TiO}_2$ Bragg reflectors centered at 550 nm are then designed: the computed photonic stopband of 477-649 nm agrees with the analytic coupled-band expression to within 1%, and the peak reflectance reaches 99.88% for 8 bilayers and 99.998% for 12 bilayers. The angular and polarization dependence of the stopband is mapped, and the reflectance spectra are connected to the Bloch band structure of the infinite crystal. Finally, a half-wave defect layer embedded in the mirror is shown to open a sharp Fabry-Perot resonance inside the stopband with a quality factor of about 1100, a resonant field enhancement of 207 inside the defect, and a spectral position tunable between 480 and 598 nm through the defect thickness. The quality factor grows exponentially with the mirror size, by a factor of 2.75 per added bilayer, and filling the defect with an analyte yields a refractometric sensitivity of 168 nm per refractive index unit, demonstrating that the presented open-source TMM framework is an efficient design tool for narrow-band optical filters and photonic sensor structures.

Keywords: Photonic crystals, transfer matrix method, Bragg reflector, defect mode, optical filter

1. INTRODUCTION

Photonic crystals are structures whose dielectric function is periodic on the scale of the optical wavelength; in analogy with electronic band theory, this periodicity opens photonic band gaps, i.e., frequency intervals in which the propagation of electromagnetic waves is forbidden [1, 2]. The one-dimensional (1D) realization of this concept, a stack of alternating high- and low-index dielectric layers, is by far the most mature member of the family: distributed Bragg reflectors provide the mirrors of vertical-cavity lasers, dielectric multilayers form the basis of interference filters and antireflection coatings, and defect-mode microcavities are exploited as narrow-band filters and label-free optical sensors [3, 6, 8].

The standard theoretical tool for such layered media is the transfer matrix method (TMM), in which each layer is represented by a 2x2 characteristic matrix and the response of an arbitrary stack follows from a simple matrix product [4, 5]. Although the method is classical, its practical value has grown with the availability of open scientific computing environments: a transparent TMM implementation of a few dozen lines of Python [9, 10] reproduces, at negligible computational cost, results that are otherwise obtained with commercial thin-film design software [6, 11]. Compared with existing open-source multilayer codes such as that of Ref. [11], the emphasis of the present framework is on verifiability: the spectra, the Bloch band structure, the internal field profiles, and the cavity figures of merit are produced within a single short script, and every quantitative output is checked against a closed-form result.

In this work, a fully open-source and analytically validated TMM framework for 1D photonic crystals is presented and applied to the complete design chain of a defect-mode optical filter. The contributions are as follows. First, the implementation is verified against four independent analytic benchmarks, with agreement at machine precision. Second, quarter-wave $\text{SiO}_2/\text{TiO}_2$ Bragg reflectors are designed systematically, and the dependence of the stopband on the number of bilayers, the index contrast, the angle of incidence, and the polarization is quantified and compared with analytic band-edge expressions. Third, the reflectance spectra are connected explicitly to the Bloch band structure of the infinite crystal, and the field localization of the defect mode is computed. Finally, the defect microcavity is characterized as a device: the tuning range, the quality factor and its exponential scaling with mirror size, and the refractometric sensitivity of an analyte-filled cavity are reported.

2. THEORY AND COMPUTATIONAL METHOD

2.1. Transfer matrix formulation. A stack of homogeneous layers $j = 1 \dots m$ with refractive indices n_j and thicknesses d_j is placed between an incidence medium n_0 and a substrate n_s . For a plane wave of vacuum wavelength λ incident at angle θ_0 , the phase thickness of layer j is

$$\delta_j = 2\pi/\lambda \cdot n_j d_j \cos \theta_j \quad (1)$$

where θ_j follows from Snell's law, and the optical admittance is $\eta_j = n_j \cos \theta_j$ for TE (s) polarization and $\eta_j = n_j / \cos \theta_j$ for TM (p) polarization. Each layer is represented by its characteristic matrix

$$M_j = \begin{bmatrix} \cos \delta_j & (i/\eta_j) \sin \delta_j \\ i\eta_j \sin \delta_j & \cos \delta_j \end{bmatrix} \quad (2)$$

and the total stack matrix is the ordered product $M = M_1 M_2 \dots M_m$. With $(B, C)^T = M(1, \eta_s)^T$, the amplitude reflection and transmission coefficients are

$$r = (\eta_0 B - C)/(\eta_0 B + C), t = 2\eta_0/(\eta_0 B + C) \quad (3)$$

from which $R = |r|^2$ and $T = (\text{Re } \eta_s / \eta_0) |t|^2$ follow [4, 5]. For the infinite periodic bilayer crystal of period $\Lambda = d_H + d_L$, the Bloch wave vector K at normal incidence obeys the dispersion relation

$$\cos(K\Lambda) = \cos \delta_H \cos \delta_L - 1/2(\eta_H/\eta_L + \eta_L/\eta_H) \sin \delta_H \sin \delta_L \quad (4)$$

whose forbidden solutions $|\cos(K\Lambda)| > 1$ define the photonic band gaps [4]. The method was implemented in Python using only the NumPy [9] and Matplotlib [10] libraries; the calculation is vectorized over wavelength, and a full spectrum of a 30-bilayer stack over 6000 wavelength points evaluates in a few milliseconds on standard desktop hardware. The quality factor of cavity resonances is defined as $Q = \lambda_{\text{res}}/\Delta\lambda$, with $\Delta\lambda$ the full width at half maximum of the transmission peak evaluated on adaptively refined wavelength grids, and the internal field distribution $|E(z)|^2$ is obtained by propagating the boundary fields from the entrance plane through the partial characteristic matrices of the traversed sublayers.

2.2. Structures and parameters. Quarter-wave Bragg mirrors $[H L]^N$ made of TiO_2 ($n_H = 2.35$) and SiO_2 ($n_L = 1.45$) on a glass substrate ($n_s = 1.52$) were designed for a center wavelength $\lambda_0 = 550$ nm, so that $d_H = \lambda_0/(4n_H) = 58.5$ nm and $d_L = \lambda_0/(4n_L) = 94.8$ nm. Defect microcavities were constructed as $(HL)^N D (LH)^N$, where the defect D is a SiO_2 layer of variable thickness d_c . All refractive indices are treated as real and nondispersive over the studied range, which is the standard idealization for design studies in the visible; material dispersion and absorption, as well as interface roughness of real films, would mainly broaden the resonances and reduce the quality factors reported below.

2.3. Validation of the implementation. Four independent analytic benchmarks were used: (i) energy conservation, $R + T = 1$, holds to better than 10^{-10} for lossless stacks at arbitrary oblique incidence; (ii) the empty stack reproduces the Fresnel reflectance of the bare air/glass interface exactly; (iii) the full spectrum of a single quarter-wave MgF_2 antireflection layer coincides with the exact single-film (Airy) formula with a maximum deviation of 5×10^{-17} , i.e., machine precision (Figure 1); and (iv) the peak reflectance of quarter-wave stacks matches the textbook closed-form expression for all tested N . Figure 1(b) also illustrates a physically instructive detail: the residual reflectance of about 1.3% at λ_0 remains because the realistic MgF_2 index ($n = 1.38$) exceeds the ideal single-layer value $(n_0 n_s)^{1/2} = 1.233$.

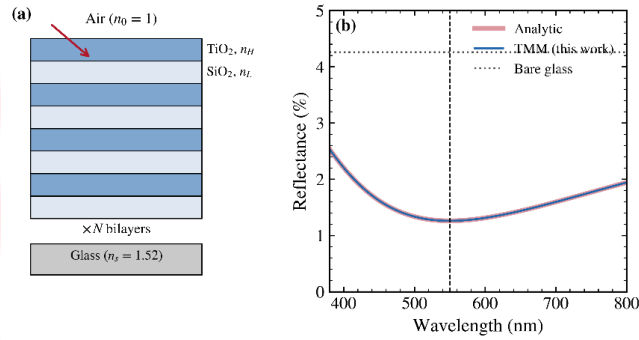


Figure 1. Method validation: (a) schematic of the studied multilayer geometry; (b) reflectance of a quarter-wave MgF_2 antireflection layer on glass computed with the present TMM implementation, overlaid on the exact single-film formula (maximum deviation 5×10^{-17}).

3. RESULTS AND DISCUSSION

3.1. Bragg reflector design. Figure 2 shows the normal-incidence reflectance of $[H L]^N$ mirrors for $N = 4, 8$, and 12 bilayers. A photonic stopband develops around λ_0 and converges rapidly toward total reflection: the numerically determined high-reflectance band, 477–649 nm (width 171 nm), agrees to within 1% with the analytic band-edge expression derived from Equation (4), shown as the shaded region. The convergence with mirror size is quantified in Figure 3(a): the transmitted remainder $1 - R_{\text{max}}$ decreases exponentially with N , in exact agreement with the closed-form quarter-wave formula, reaching $R_{\text{max}} = 99.88\%$ for $N = 8$ and 99.998% for $N = 12$. Figure 3(b) shows that the stopband width grows monotonically with the index contrast n_H/n_L and follows the analytic arcsin-dependence over the whole studied range; the $\text{TiO}_2/\text{SiO}_2$ pair (contrast 1.62) already provides a bandwidth covering one third of the visible spectrum.

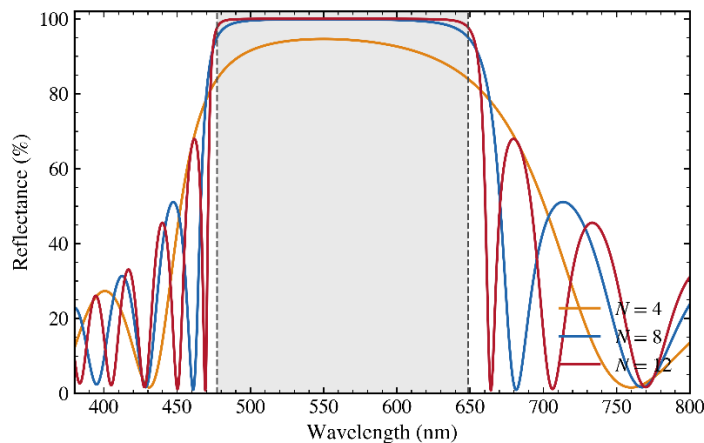


Figure 2. Normal-incidence reflectance of $[HL]^N$ Bragg mirrors for $N = 4, 8$, and 12 bilayers. The shaded region marks the analytic photonic stopband obtained from Equation (4).

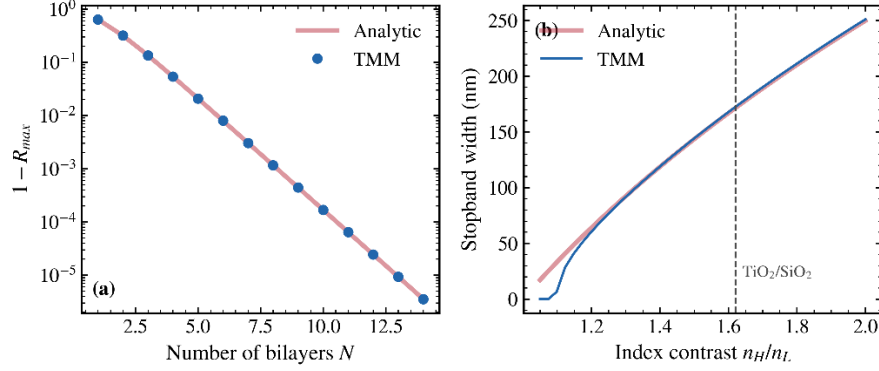


Figure 3. (a) Exponential decrease of $1 - R_{\max}$ with the number of bilayers, compared with the closed-form quarter-wave expression; (b) stopband width versus index contrast n_H/n_L , compared with the analytic arcsin law.

3.2. Angular and polarization response. Figure 4 maps the reflectance of the $N = 8$ mirror as a function of wavelength and angle of incidence for both polarizations. The stopband shifts toward shorter wavelengths with increasing angle, as expected from the reduction of the effective optical path $n d \cos\theta$, and the two polarizations split: the TE gap remains wide up to grazing incidence, whereas the TM gap narrows appreciably because the TM admittance contrast collapses in the vicinity of the internal Brewster condition. This polarization asymmetry is the reason why omnidirectional reflection in 1D crystals requires sufficiently high index contrast and a suitably placed band [7]; for the present material pair, the $N = 8$ mirror maintains $R > 99\%$ for both polarizations over the central part of the stopband for angles up to about 50 degrees.

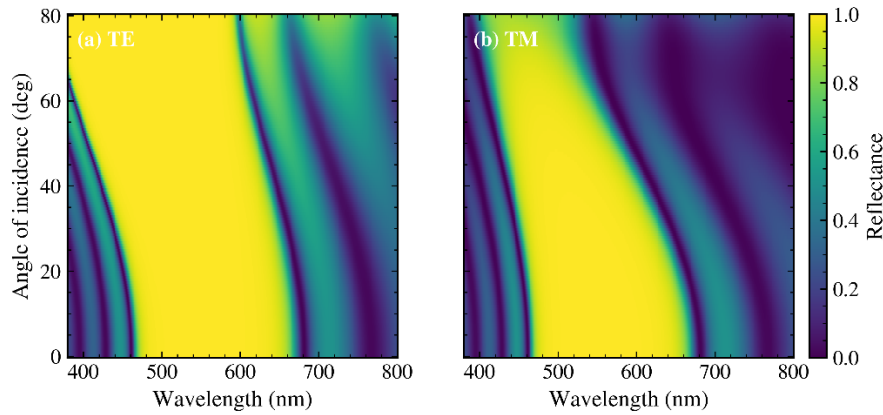


Figure 4. Angle-resolved reflectance maps of the $N = 8$ mirror for (a) TE and (b) TM polarization, showing the blueshift of the stopband and the polarization splitting at oblique incidence.

3.3. Band structure and field localization. The connection between the finite-stack spectra and the physics of the infinite crystal is made explicit in Figure 5(a), which shows the Bloch band structure obtained from Equation (4): the design wavelength $\lambda_0 = 550$ nm lies in the center of the first photonic band gap, and the higher-order gaps at $\Lambda/\lambda \approx 0.8$ and 1.4 correspond to the secondary reflection bands of the finite mirrors. Figure 5(b) shows the normalized field intensity $|E(z)|^2$ inside the defect microcavity. On resonance, the field grows exponentially through the mirrors and reaches an enhancement of 207 relative to the incident intensity inside the defect layer, whereas 20 nm away from the resonance it decays evanescently by more than five orders of magnitude across the same structure. This strong and spatially selective enhancement is precisely the property exploited in cavity-enhanced spectroscopy and sensing applications [8].

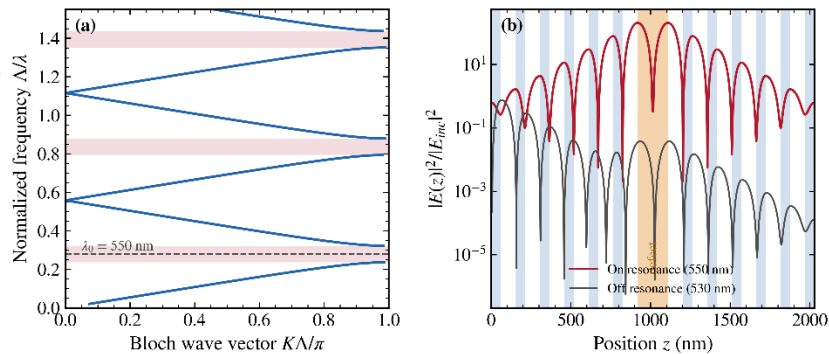


Figure 5. (a) Bloch band structure of the infinite $\text{TiO}_2/\text{SiO}_2$ crystal at normal incidence; shaded bands mark the photonic gaps and the dashed line the design wavelength. (b) Normalized field intensity $|E(z)|^2$ inside the defect microcavity on and off resonance; the defect layer is highlighted.

3.4. Defect-mode filter and its tuning. Figure 6(a) shows the transmittance of the $(\text{HL})^6 \text{D} (\text{LH})^6$ cavity for three defect thicknesses: a single sharp Fabry-Perot resonance appears inside the otherwise opaque stopband, with near-unity peak transmission. For the half-wave defect ($d_c = \lambda_0/2n_c$) the resonance falls exactly at 550.0 nm with a quality factor $Q \approx 1100$. Figure 6(b) demonstrates the tuning law: the resonance wavelength shifts linearly with the defect thickness over the range 480-598 nm, i.e., across essentially the whole stopband, while Q passes through a maximum near the half-wave condition. At $d_c n_c / \lambda_0 \approx 0.68$ the resonance jumps back to the short-wavelength band edge, marking the entry of the next longitudinal cavity mode into the stopband.

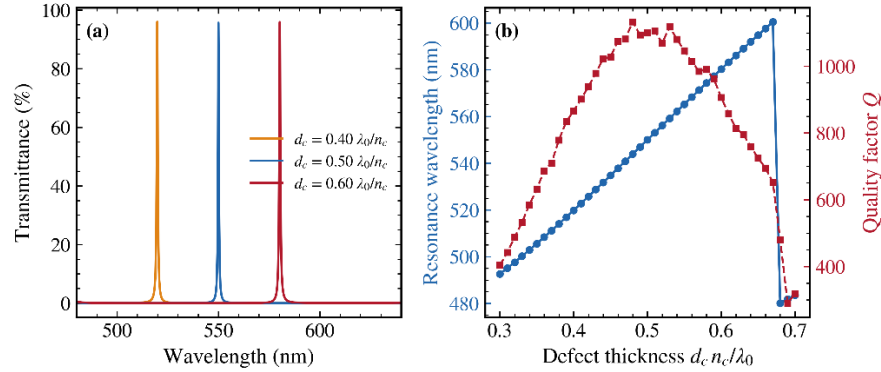


Figure 6. (a) Transmittance of the defect microcavity for three defect thicknesses; (b) resonance wavelength (left axis) and quality factor (right axis) versus normalized defect thickness.

3.5. Cavity scaling and refractometric sensing. Figure 7(a) shows that the quality factor grows exponentially with the number of mirror bilayers, $Q \propto e^{1.01N}$, i.e., each added bilayer multiplies Q by 2.75, from $Q = 55$ at $N = 3$ to $Q = 9387$ at $N = 8$. This behavior directly reflects the exponential decrease of the mirror transmission established in Figure 3(a) and provides a simple design rule for target linewidths. As an application, Figure 7(b) considers a sensing configuration in which the defect layer of fixed physical thickness (200 nm), embedded between $N = 5$ bilayer mirrors, is filled with an analyte of refractive index n_c between 1.30 and 1.45: the resonance wavelength shifts linearly with a refractometric sensitivity of $S = d\lambda/dn = 168 \text{ nm/RIU}$, a value of the same order as the sensitivities reported for porous-silicon photonic crystal microcavity sensors [8, 12]. In practice, such an analyte-accessible defect corresponds to porous-layer or open flow-cell microcavity architectures rather than to a monolithic dielectric stack [12]. Table 1 summarizes the key quantitative results of the study.

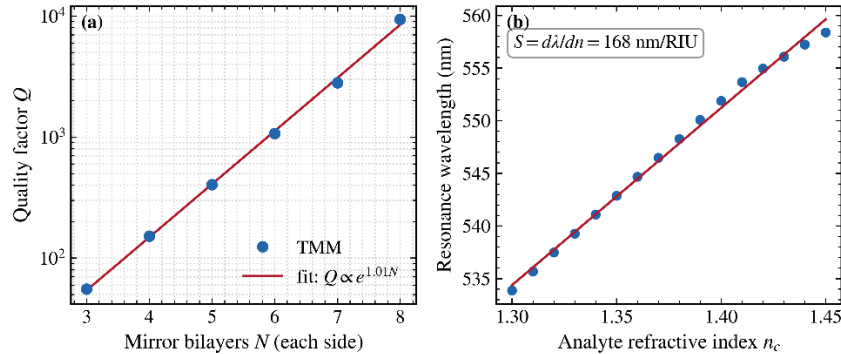


Figure 7. (a) Quality factor versus number of mirror bilayers with exponential fit; (b) resonance wavelength versus analyte refractive index in the sensing configuration, with linear fit giving $S = 168 \text{ nm/RIU}$.

Table 1. Summary of the key quantitative results

Quantity	Value
Validation: max. deviation from analytic single-film spectrum	5×10^{-17}
Photonic stopband ($\text{TiO}_2/\text{SiO}_2$, $\lambda_0 = 550 \text{ nm}$)	477-649 nm (171 nm)
Peak reflectance, $N = 8 / N = 12$ bilayers	99.88% / 99.998%
Defect resonance (half-wave, $N = 6$): wavelength / Q	550.0 nm / ≈ 1100
Resonant field enhancement in the defect	207
Tuning range via defect thickness	480-598 nm
Q scaling with mirror size	$Q \propto e^{1.01N}$ ($\times 2.75$ per bilayer)
Refractometric sensitivity (analyte-filled defect)	168 nm/RIU

The main limitations of the present treatment are the neglect of material dispersion and absorption and, for the band-structure analysis, the restriction to normal incidence. In realistic sputtered or evaporated films, scattering and absorption losses impose an upper bound on the achievable Q , so the exponential scaling of Figure 7(a) holds until the mirror transmission becomes comparable to the round-trip loss. Including measured dispersion data and complex indices in Equations (1)–(3) is straightforward within the same framework and is a natural next step, as is the extension to oblique-incidence band structures and to aperiodic or chirped multilayers.

4. CONCLUSION

A compact, fully open-source transfer matrix framework for one-dimensional photonic crystals has been presented and validated against four analytic benchmarks at machine precision. Applied to quarter-wave $\text{SiO}_2/\text{TiO}_2$ mirrors at 550 nm, the framework reproduces the analytic stopband (477-649 nm) to within 1% and quantifies the exponential convergence of the reflectance with mirror size (99.998% at 12 bilayers). The finite-stack spectra were connected to the Bloch band structure of the infinite crystal, and a half-wave defect layer was shown to create a high-quality Fabry-Perot resonance ($Q \approx 1100$, field enhancement 207) that is tunable across the entire stopband through the defect thickness. The quality factor scales as $Q \propto e^{1.01N}$, and an analyte-filled cavity exhibits a refractometric sensitivity of 168 nm/RIU. The complete study runs in about one minute on free cloud hardware, demonstrating that analytically validated open-source tools are fully sufficient for the quantitative design of narrow-band photonic crystal filters and sensor structures.

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F-4

DETERMINING THE FINANCIAL BEHAVIOR PROFILES OF CONSTRUCTION INSPECTION STUDENTS USING DECISION TREES AND CLUSTER ANALYSIS**Ahmet Onay^{1,*}, Utku Kaya²**¹ Vocational School of Transportation, Eskisehir Technical University, 26140 Eskişehir, Türkiye² Vocational School of Transportation, Eskisehir Technical University, 26140 Eskişehir, Türkiye**ABSTRACT**

The increase in average life expectancy, demographic changes in society, and the diverse behavioral characteristics of individuals are creating global pressure on the sustainability of traditional public social security systems, a pressure that also significantly affects Turkey. To alleviate this pressure and achieve the macroeconomic fund accumulation goal underlined in the 12th Development Plan, the government and public authorities are implementing various tools. The individual retirement system and its extension, the automatic enrollment system, are particularly aimed at encouraging young people to develop saving habits at an early age. This study, contrary to the general trend in the literature, investigates the financial tendencies of students in a technical associate degree program. The main objective of this study is to reveal the structural financial behavior profiles of associate degree students by analyzing their participation tendencies in the retirement system, their knowledge levels, and their trust attitudes towards the system using machine learning algorithms. In the analysis of the dataset, decision tree algorithms were used to create a predictive model, and hierarchical clustering algorithms were used to divide students into homogeneous financial groups. The findings from the decision tree analysis show that the most dominant determinant of students' decision to participate in the individual retirement system is household income. Furthermore, findings showed that construction supervision students in the lower-middle income group differed dramatically from the control group. Hierarchical clustering analysis revealed that the students were divided into three distinct financial profiles. These findings have the potential to contribute to the development of specific policy interventions based on behavioral finance.

Keywords: Financial Literacy, Decision Trees, Clustering Analysis, Retirement System.

1. INTRODUCTION

One of the most significant consequences of increasingly comfortable living conditions for humankind is the extension of life expectancy. This increase in life expectancy is the primary factor causing demographic aging. However, from the perspective of public pension systems, this situation is one of the most important macroeconomic factors threatening the sustainability of the system [1]. Many countries are designing and implementing various structural reforms to control this systemic risk. Chief among these are regulations encouraging individuals to participate in voluntary or automatic private pension systems. In Turkey, the individual pension system, which has a long history, is encouraged by the public authority through various regulations. The automatic enrollment system, which came into effect on January 1, 2017, and the supplementary pension system (TES), planned to be implemented in the coming days, are important steps taken by the public authority to ensure the sustainability of the pension system. Despite numerous government incentives and regulatory interventions, the integration of citizens into these systems is not solely dependent on rational economic decisions. Citizens' levels of financial literacy, cognitive limitations, and behavioral tendencies are among the dominant factors shaping their integration into the system. In this context, it can be said that the literature has developed around three main axes. These are financial literacy, behavioral finance, and studies based on machine learning algorithms, which are actually a combination of the two and have been used in recent years to identify these trends.

The concept of financial literacy is a strong theoretical foundation behind studies examining individuals' long-term financial planning and retirement savings decisions. One of the most fundamental conclusions of a comprehensive literature review by [2] is that individuals with higher levels of financial literacy are significantly more likely to plan for retirement and more successful in implementing those plans. Another study focusing on the impact of financial knowledge on participation in complex financial instruments by [3] confirms this conclusion. According to this study, individuals lacking basic financial literacy have lower risk tolerances and move away from retirement systems towards traditional, low-return savings methods. Low levels of financial knowledge lead individuals to invest in more secure and less informative investments. Global research specifically on young adults and university students shows that financial knowledge is insufficient in this age group. It has been confirmed that those in this age group do not fully understand fundamental elements of long-term saving, such as inflation, compound interest, and risk diversification [4].

On the other hand, a lack of knowledge about financial matters alone is insufficient to explain individuals' participation in long-term savings instruments such as retirement systems. In other words, a significant portion of individuals' financial behavior can only be explained from a behavioral finance perspective, which challenges the homo economicus assumption of traditional financial theories that investment decisions are rational. Behavioral finance focuses on psychological biases in financial decision-making processes. Many psychological factors affecting human beings influence the shaping of investment decisions. For example, within the context of Loss Aversion, proposed under Prospect Theory [5], individuals are more sensitive to present losses—more specifically, to a clearer example, an immediate decrease in disposable income—than to the benefits they will receive in the future. Especially in the context of individual retirement planning, the present bias is a known problem, leading individuals to constantly postpone their savings decisions. Public pension schemes can turn these concerns addressed by behavioral finance theories into an advantage. [6] demonstrated how auto-enrollment systems, designed to leverage individuals' inertia and status quo deviations, radically increase

retirement savings. The theoretical foundations of this regulation, which is also implemented in Türkiye, are based on behavioral finance theories.

Although the vast majority of financial behavior research in the current literature relies on classical statistical and parametric models, the use of machine learning algorithms in revealing financial behavior profiles has become increasingly common in recent years. The main reason for the prominence of machine learning algorithms is that traditional statistical methods model human behavior in a linear context and fail to adequately capture the underlying relationships. However, individuals' financial behavior is based on complex, multi-layered relationships between socio-demographic factors and psychological attitudes. Machine learning algorithms have a much higher potential than traditional methods in separating individual investors according to their financial decision-making styles and psychological biases. [7] laid the foundation for the use of clustering approaches for this purpose. Unsupervised learning algorithms such as hierarchical clustering and K-means, unlike traditional statistical methods, do not force investors into predefined categories. Thanks to these methods, homogeneous behavioral profiles based on natural mathematical similarities within the data itself can be revealed [8]. On the other hand, decision trees stand out in mapping the nonlinear and hierarchical effects of independent variables on the target variable. With this methodology, for example, individuals' decision to participate in the retirement system can be mapped as a target variable. Studies by [9, 10, 11, 12] have shown that decision trees offer higher accuracy and excellent visual interpretability in predicting financial trends compared to traditional logistic regression models.

This study reveals the financial behavior and perceptions of construction supervision students, a technical associate degree program, using clustering approaches and decision tree algorithms. Numerous studies exist in the Turkish literature examining university students' perceptions of the individual retirement system, particularly due to the ease of access to samples. However, these studies have generally focused on social science students and have been limited to measuring awareness levels using classical survey methods. This study is expected to contribute to the literature in two ways. Firstly, it examines the financial tendencies of technical associate degree students in an analytical and field-oriented education, combining rational knowledge levels with behavioral trust attitudes through a sample. Secondly, it utilizes data mining algorithms such as Decision Trees and Hierarchical Clustering instead of the parametric assumptions frequently used in the literature.

2. METHODOLOGY AND DATA ANALYSIS

A correlational survey model was used to identify the relationships, patterns, and effect levels between the variables in the research model. The research population consisted of associate degree students studying at Eskişehir Technical University. The sample included students from the construction inspection program (n=44), a technical associate degree program, in the context of the research objective. Additionally, students from the logistics program (n=29) were included as a control group. This group was added to the sample to clearly observe the impact of different disciplines on financial decision-making processes in machine learning algorithms.

The research data was collected through a survey form designed in accordance with the research objective. The survey form consists of three sections:

1. Demographic Characteristics: This section comprises categorical questions aimed at determining characteristics such as the students' field of study, gender, grade level, and average monthly household income range.
2. Measuring Knowledge Level Regarding the System: This section consists of 5 multiple-choice questions (True/False/No Opinion) measuring individuals' objective knowledge of the system's operation, government contributions, exit rights, and fund security.
3. Measuring Trust in the System: The questions in this section aim to measure the students' level of trust in official authorities, private pension companies, macroeconomic stability (the most important determinant being protection against inflation), and legal security, the most fundamental component of the system. This section consists of 6 questions using a 5-point Likert scale (1: Strongly Disagree - 5: Strongly Agree). On the other hand, this section also includes a binary question (Yes/No) measuring the tendency to participate in the individual retirement system, which is the target variable of the research.

The following questions aim to measure the level of knowledge regarding the Private Pension System (BES). The options for answering these questions are true, false, and I have no opinion. These questions are designed to understand whether students are aware of the system's features.

BD1. In the Individual Retirement System, the state provides additional contributions to the amount invested by participants.

BD2. To be eligible for retirement benefits from BES, it is mandatory to remain in the system for at least 10 years and reach the age of 56.

BD3. Funds accumulated in BES accounts are invested only in government bonds; participants do not have the right to choose their investment vehicle.

BD4. Employees included in the system by their employer under the Automatic Enrollment System have the right to withdraw from the system at any time.

BD5. In the event of the retirement company's bankruptcy, the funds of BES participants may be seized or garnished to cover the company's debts.

The questionnaires designed to measure students' level of trust in the system are presented below. These questions are designed as 5-option Likert-type questions. Students' level of trust in the system is a multidimensional variable and is influenced by various factors. In this context, it is necessary to measure trust in the government, trust in the private pension company, and trust in the macroeconomy separately, and the scale items are designed to measure these three different dimensions.

G1. I trust the official institutions that regulate and supervise the Private Pension System.

G2. I believe that private pension companies will manage my savings transparently and honestly.

G3. I am confident that I will be able to withdraw my savings and returns from the Private Pension System without any problems in the long term.

G4. I believe that the government will continue to maintain the current contribution incentive program steadily in the future.

G5. I believe that my investments in the Private Pension System are legally protected and will not be seized even during periods of economic fluctuation or crisis.

G6. I believe that the returns on the funds in the Private Pension System will protect my savings against inflation in the long term.

The raw data obtained from the research were cleaned and prepared for analysis before the analysis. Orange Data Mining 3.4 was used for the analyses. The decision tree algorithm was used to reveal the nonlinear and hierarchical effects of independent variables on the target variable. In this process, it was determined that the perception of trust in the system alone distinguished 100% of the students' decisions. Therefore, to prevent overfitting and masking of sub-components in the model, the trust variables were excluded from the model and the analysis continued. This new decision tree model directly focuses on socio-economic and interdisciplinary patterns. In the second stage of the analysis, the hierarchical clustering algorithm was applied to separate the students into homogeneous profiles based on the mathematical similarities of their responses to the variables of knowledge about the system, trust in the system, and demographic variables, independently of any target variable.

3. FINDINGS

Figure 1 presents a decision tree model created to map the hierarchical structure of factors predicting participants' attitudes towards the individual retirement system.

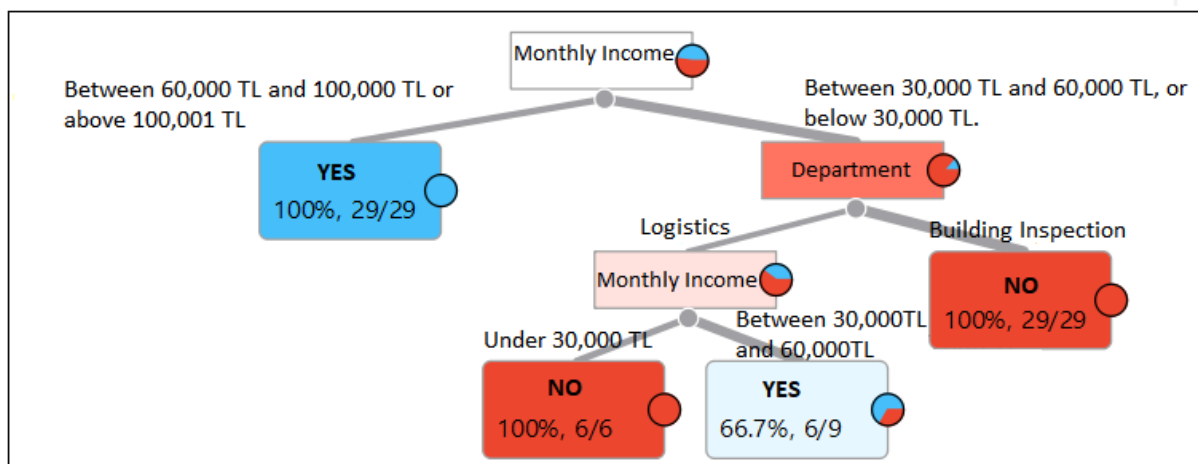


Figure 1. Decision Tree Model of the Study

Figure 1 visualizes the factors determining students' tendency to participate in the Private Pension System (BES). Examining the figure, it can be seen that the decision tree algorithm divides the entire dataset into two groups based on the monthly income variable. Accordingly, all 29 students who participated in the survey, regardless of their educational program, and whose household income is 60,000 TL or more, stated that they would participate in the BES. This finding shows that, contrary to the general trend in the literature, the biggest obstacle to entering the system is not a lack of knowledge or awareness about the system. According to our findings, the most fundamental difficulty in entering the BES is directly insufficient disposable income. The second and most striking breakdown of the model is visualized on the right side of the figure. In this breakdown, the decision tree algorithm separated the group with income below 60,000 TL according to the program variable. All students in the construction inspection program refused to enter the system under this income constraint. In contrast, despite being in the same income group, students in the logistics program showed a tendency to participate in the BES at a rate of 66.7% (6/9). This sharp difference can be interpreted as the logistics program curriculum providing long-term planning, cost analysis, and rational process management skills, enabling students to demonstrate financial resilience and a saving reflex even under low budget constraints. Alternatively, students in the building inspection program may consider their financial situation more when making decisions about their finances, or the extra expenses required for the technical section when their income level falls below 60,000 TL may force them into this financial behavior.

In the Hierarchical Clustering analysis, students' demographic characteristics, knowledge levels regarding the retirement system, and confidence scores about the system were evaluated as a whole and grouped using mathematical distance metrics. The dendrogram graph of this grouping is presented in Figure 2. By determining the split point at the distance level of 10, 3 main profiles (C1, C2, C3) reflecting the basic behavioral characteristics of the dataset were obtained. By evaluating the clusters obtained as a result of the analysis, the 3 profiles formed by the students were defined.

Blue Cluster (Financial Skeptics): According to the analysis results, this group comprises the largest number of students and is represented by the highest volume in the graph. Students in this group consist of participants with low income levels, who scored poorly on the knowledge test about private pension schemes (BES), and who have deep distrust of the pension system, particularly in terms of its protection against inflation. All students in this group expressed a "No" opinion regarding participation in BES. This finding can be interpreted as macroeconomic uncertainties completely halting long-term planning.

Red Group (Analytical and Informed Investors): The red group consists of students willing to enter the retirement system. This group is predominantly comprised of Logistics program students. These students are the ones who give the most accurate answers to technical details such as fund management and the right of withdrawal. It can be said that this group trusts the retirement system's features such as government incentives, stability, and the transparency of private companies. It can be argued that this is the most rational group.

Green Cluster (State-Oriented Traditionalists): While students in this cluster are willing to enter the retirement system, they exhibit a profile that differs from the red cluster. This group mostly consists of students from the Construction Inspection program. They have limited knowledge of technical aspects of the retirement system, such as fund types, and approach private sector retirement companies with suspicion. However, their high level of trust in the official authority, legal guarantees, and features of the system such as state contributions leads these students to accept integration into the system. Behaviorally, this group is motivated not by their level of knowledge, but by state authority and guarantees.

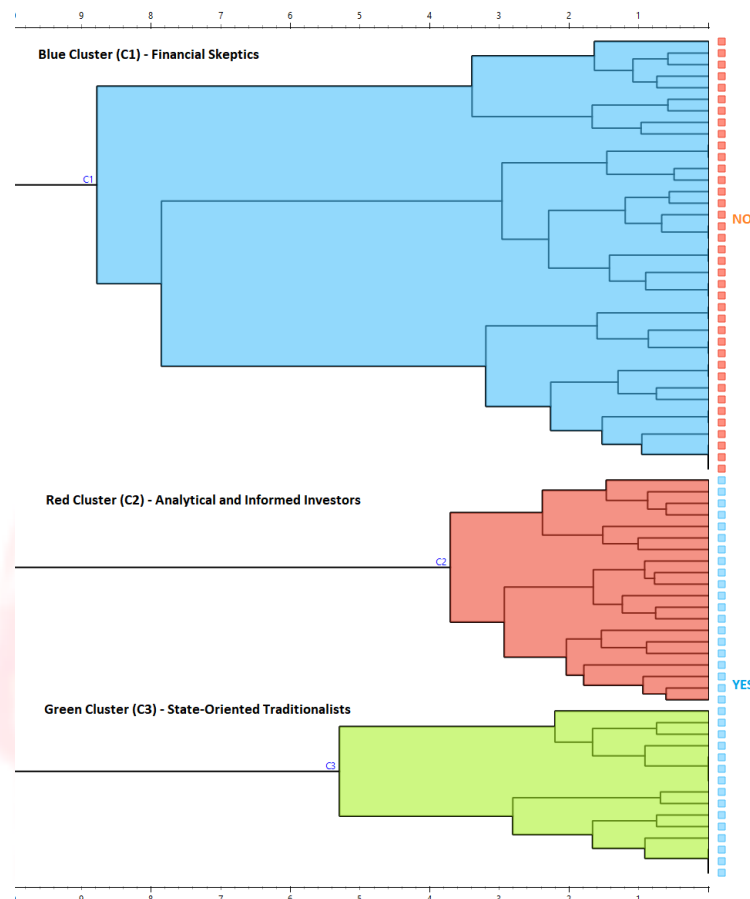


Figure 2. Hierarchical Clustering Dendrogram Based on Financial Behavior

4. CONCLUSION

This study examines the tendency of young individuals to participate in the Private Pension System, designed as a supplementary security mechanism, during a period of increasing demographic and economic pressures on social security systems. The findings, obtained using Decision Trees and Hierarchical Clustering algorithms, demonstrate that individuals' long-term financial planning decisions are influenced by a complex interplay of financial literacy levels, socioeconomic constraints, the cognitive foundation acquired through education, and psychological attitudes towards the system.

The decision tree showed that the absolute determinant of the decision to participate in the Private Pension System (BES) is household income level. The fact that all students with an average monthly income above 60,000 TL showed a willingness to participate in the system reveals that the main obstacle to the integration of young people into savings systems is financial inadequacy. This finding indicates that the level of knowledge and awareness, which would be expected to be the primary obstacle, is actually secondary or tertiary. On the other hand, a sharp interdisciplinary divide was observed in the lower-middle income group. In this group, unlike the students in the control group, all students in construction supervision refused to save. This shows that having different competencies affects individuals' investment decisions.

Hierarchical clustering analysis revealed that students were divided into three distinct financial profiles. The group we call financial skeptics consists of those who prefer to remain completely outside the system. The group we call analytical and informed investors participate, trusting in the system's characteristics to a certain extent. The last group, which we call state-focused traditionalists, is motivated by legal guarantees and government incentives.

The findings of this study serve to develop some recommendations for policymakers. First, the findings point to the importance of financial education tailored to the target audience. In particular, in training for students in technical and field-oriented areas such as

building inspection, the use of complex fund management terminology should be limited, and the legal security of the system and simple savings steps should be emphasized. For the profile of financial skeptics, the problem was found to be trust and income constraints. This finding indicates that arrangements similar to the Automatic Enrollment System (AES) are effective on this group. Furthermore, behavioral nudges, such as digital banking solutions that transfer fractional amounts of spending to the Private Pension System, are likely to be effective on this group. Finally, the findings also reveal that curriculum revisions incorporating financial literacy can be effective. This is because the control sample, who already took financial literacy courses, showed a higher tendency to participate in the BES due to their level of knowledge.

The most significant limitation of this study is that its sample is limited to students in an associate degree program at a single university. Future research could extend the machine learning approaches used in this study to larger samples, different universities, and especially to young professionals already actively involved in the system. This would provide a deeper understanding of financial decision-making mechanisms. The methodology and profile decomposition technique of this study will serve as a guide for future research.

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THEORETICAL INVESTIGATION OF THE STRUCTURAL, ELECTRONIC, AND VIBRATIONAL PROPERTIES OF 8-CHLOROTHEOPHYLLINE USING DFT AND TD-DFT METHODS

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ABSTRACT

8-Chlorotheophylline (CTP) is a xanthine derivative of considerable pharmaceutical importance due to its application in medicinal chemistry and drug formulations. In this study, the structural, electronic, and vibrational properties of 8-chlorotheophylline were theoretically investigated using Density Functional Theory (DFT) and Time-Dependent Density Functional Theory (TD-DFT). All calculations were carried out at the B3LYP/6-311++G(d,p) level of theory. The optimized molecular geometry was confirmed as a true minimum by the absence of imaginary vibrational frequencies. Geometrical parameters and vibrational frequencies were analyzed to characterize the molecular structure and identify the fundamental vibrational modes.

The electronic properties of the molecule were examined through frontier molecular orbital (HOMO–LUMO) analysis, and quantum chemical descriptors such as the energy gap, ionization potential, electron affinity, chemical hardness, softness, electronegativity, and electrophilicity index were determined. In addition, Molecular Electrostatic Potential (MEP) analysis was performed to identify the most probable reactive regions of the molecule. The electronic absorption spectrum was investigated using TD-DFT calculations, and the main electronic transitions were interpreted in terms of excitation energies, oscillator strengths, and orbital contributions. The theoretical results provide a comprehensive understanding of the molecular structure, stability, electronic behavior, and spectroscopic properties of 8-chlorotheophylline, offering useful reference data for future experimental and pharmaceutical studies.

Keywords: 8-Chlorotheophylline; Density Functional Theory (DFT); Time-Dependent Density Functional Theory (TD-DFT); Molecular Electrostatic Potential (MEP); HOMO–LUMO Analysis.

1. INTRODUCTION

Xanthine and methylxanthine derivatives constitute an important class of purine-based heterocyclic compounds with considerable pharmaceutical and biological significance. Among these compounds, theophylline (1,3-dimethylxanthine) has been extensively investigated because of its bronchodilatory, anti-inflammatory, and central nervous system stimulant properties, and it has been widely used in the treatment of respiratory disorders [1–3]. Theophylline and related methylxanthines exhibit diverse structural, electronic, and intermolecular interaction properties that are closely associated with their biological activity and pharmaceutical behavior [4]. Vibrational spectroscopy combined with quantum chemical calculations has been successfully employed to characterize the molecular structure, bonding properties, charge-transfer interactions, and hydrogen-bonding behavior of methylxanthine derivatives [5,6]. In particular, Sheeba Sherlin et al. investigated 1,3-dimethylxanthine using FT-IR, FT-Raman spectroscopy and DFT calculations at the B3LYP/6-311++G(d,p) level, and identified characteristic vibrational bands associated with the xanthine ring and carbonyl groups. Their study further demonstrated the relevance of dipole moment, charge-transfer interactions, and non-covalent interactions to the biological behavior of theophylline [6]. Hirshfeld-surface analysis and DFT studies of pharmaceutically relevant methylxanthines, including theophylline, have also demonstrated the importance of hydrogen bonding and other intermolecular contacts in determining their crystal packing and structural properties [7].

The structural and spectroscopic behavior of theophylline has also been investigated in isolated and hydrated environments. Singh reported that hydrogen bonding with water molecules, particularly at the carbonyl sites, significantly influences the vibrational and electronic properties of theophylline and can modify its electronic excitation energies [8]. In another theoretical study, 8-substituted methylxanthines were investigated using DFT calculations, demonstrating that substitution at the 8-position can substantially modify the physicochemical and spectral characteristics of the xanthine framework [9]. More specifically, Prabavathi and Senthil Nayagi reported a detailed spectroscopic and DFT investigation of 8-chlorotheophylline, including FT-IR, FT-Raman, NMR, first-order hyperpolarizability, and frontier molecular orbital analyses [10]. In addition, recent computational investigations of halogen-substituted aromatic systems have shown that halogen substitution can alter the frontier molecular orbital energies and reduce the HOMO–LUMO energy gap, thereby affecting molecular reactivity [11]. These findings suggest that replacement of the hydrogen atom at the C8 position of theophylline by chlorine may produce significant changes in its molecular geometry, vibrational characteristics, electronic structure, and reactivity. Therefore, in the present work, the structural, electronic, vibrational, and optical properties of 8-chlorotheophylline are systematically investigated using DFT and TD-DFT calculations at the B3LYP/6-311++G(d,p) level. The calculated results are compared with previously reported theoretical data for 8-chlorotheophylline and the parent theophylline molecule in order to elucidate the effects of chlorine substitution on the physicochemical and spectroscopic properties of this pharmaceutically relevant xanthine derivative.

2. OPTIMIZED GEOMETRY

The structural and electronic properties of 8-chlorotheophylline (CTP) were investigated using density functional theory (DFT) calculations at the B3LYP/6-311++G(d,p) level. All calculations were performed using the Gaussian 09 program package [12]. The molecular geometry was fully optimized without imposing any constraints on the geometrical parameters. The optimized structure obtained from the geometry optimization was subsequently used for the vibrational frequency analysis.

The optimized geometry of CTP corresponds to a stable minimum on the potential energy surface, with a calculated total electronic energy of -1100.847 Hartree. The absence of imaginary vibrational frequencies confirms that the optimized structure represents a true minimum-energy configuration rather than a transition-state structure. The labeling scheme adopted for the optimized molecular structure is presented in Fig. 1.

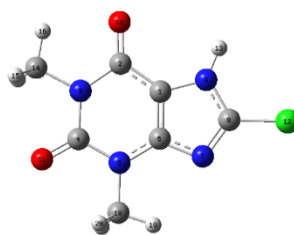


Figure1. The labeling scheme adopted for the optimized molecular structure

The calculated geometrical parameters provide important information about the structural characteristics of the molecule. In particular, the calculated C8–C12 bond length is 1.7171 Å, indicating the characteristic bonding environment associated with these atoms in the optimized structure. The remaining optimized bond lengths and bond angles are summarized in Table 1. The optimized structural parameters obtained at the B3LYP/6-311++G(d,p) level provide the basis for the subsequent analysis of the vibrational, electronic, and nonlinear optical properties of CTP.

Table 1. Optimized geometrical parameters of CTP calculated at the B3LYP/6-311++G(d,p) level

Bond length	Value (Å)	Bond angle	Value (°)	Torsional angle	Value (°)
N1–C2	1.4075	N1–C2–N3	117.27	N1–C2–N3–C4	0
C2–N3	1.3940	C2–N3–C4	118.18	C2–N3–C4–C5	0
N3–C4	1.3713	N3–C4–C5	126.84	N3–C4–C5–C6	0
C4–C5	1.3755	C4–C5–C6	119.49	C4–C5–C6–N1	0
C5–C6	1.4301	C5–C6–N1	111.69	C5–C6–N1–C2	0
C6–N1	1.4168	C6–N1–C2	126.71	C6–N1–C2–N3	0
C4–N7	1.3652	C4–N7–C8	105.17	C4–N7–C8–N9	0
N7–C8	1.3163	N7–C8–N9	113.85	N7–C8–N9–C5	0
C8–N9	1.3545	C8–N9–C5	104.92	C8–N9–C5–C4	0
N9–C5	1.3863	N9–C5–C4	110.33	N9–C5–C4–N7	0
C10–N1	1.4691	C5–C4–N7	106.28	C5–C4–N7–C8	0
O11–C2	1.2169	C10–N1–C6	117.44	C10–N1–C6–C5	180
C12–N3	1.4655	O11–C2–N1	122.46	C6–N1–C2–O11	180
N7–H13	1.0093	C12–N3–C2	119.80	N1–C2–N3–C12	180
C10–H15	1.0902	H13–N7–C4	128.47	N3–C4–N7–H13	0
C10–H16	1.0863	N7–C8–C112	119.74	C4–N7–C8–C112	180
C10–H17	1.0902	N9–C5–C6–O15	127.14	N9–C5–C6–O15	0
C12–H19	1.0872	N1–C10–H15	107.26	C6–N1–C10–H15	0
C12–H20	1.0903	N1–C10–H16	110.04	C6–N1–C10–H16	120
C12–H21	1.0904	N1–C10–H17	110.04	C6–N1–C10–H17	–120

The calculated dipole moment of CTP is 2.291727 D. The non-zero dipole moment indicates an asymmetric distribution of electronic charge within the molecule and reflects the combined contribution of the heteroatoms and the molecular substitution pattern. This result is particularly relevant for understanding the molecular electrostatic properties and the interaction of CTP with its surrounding environment. The calculated dipole moment will also be useful in interpreting the molecular electrostatic potential and nonlinear optical properties discussed in the following sections.

The B3LYP functional combines Becke's three-parameter exchange functional with the Lee–Yang–Parr correlation functional and has been widely employed for the investigation of molecular structures and vibrational properties [13–15]. The 6-311++G(d,p) basis set includes diffuse and polarization functions, which are particularly useful for describing the electron distribution and molecular properties of systems containing heteroatoms. Therefore, the B3LYP/6-311++G(d,p) level was selected as an appropriate computational approach for the present investigation.

Overall, the optimized structural parameters and the calculated dipole moment demonstrate that the CTP molecule possesses a well-defined stable molecular structure. The optimized geometry obtained here was subsequently employed in the vibrational frequency, frontier molecular orbital, molecular electrostatic potential, and other electronic-property analyses.

3. VIBRATIONAL ENERGY ANALYSIS

The vibrational properties of 8-chlorotheophylline (CTP) were investigated at the B3LYP/6-311++G(d,p) level using the Gaussian 09 program package. Following geometry optimization, harmonic vibrational frequency calculations were performed for the optimized structure. The calculated vibrational frequencies were used to characterize the normal modes of CTP and to assign the

major infrared (IR) absorption bands. The absence of imaginary frequencies confirms that the optimized molecular structure corresponds to a true minimum on the potential energy surface. The calculated vibrational frequencies and their assignments were compared with the previously reported experimental and theoretical results of Prabavathi and Senthil Nayaki [10], who investigated 8-chlorotheophylline using DFT calculations at the B3LYP/6-311++G(d,p) level together with FT-IR and FT-Raman spectroscopy is shown in Fig.2. The comparison shows good overall agreement between the present calculations and the previously reported spectral data.

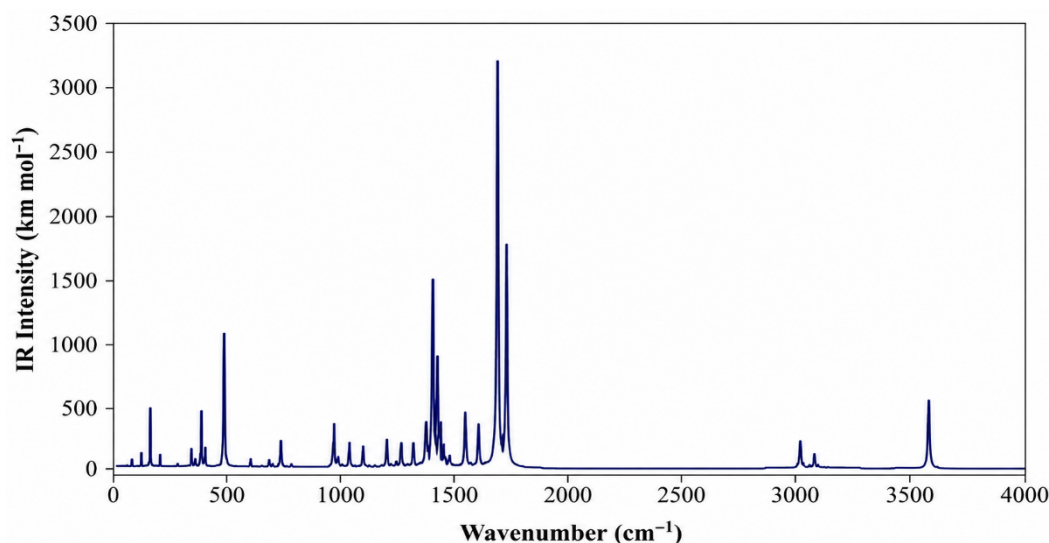


Figure 2. Calculated infrared (IR) spectrum of 8-chlorotheophylline obtained at the B3LYP/6-311++G(d,p) level of theory.

The most important calculated IR-active modes are presented in Table 2. In the low-frequency region, the calculated band at 500.65 cm^{-1} , with a relatively high IR intensity of 87.07 km mol^{-1} , is assigned mainly to C–H out-of-plane bending vibrations. The calculated band at 701.4 cm^{-1} can be assigned predominantly to C–Cl stretching vibrations and is in good agreement with the previously reported value of approximately 700 cm^{-1} . The calculated bands at 1058.7 and 1120.4 cm^{-1} are mainly associated with C–N stretching and ring vibrations, while the band at 1226.9 cm^{-1} is related to C–N/ring stretching contributions. These calculated values are consistent with the corresponding bands reported in the previous study. In the middle-frequency region, several relatively intense bands are observed. The calculated bands at 1344.5 and 1429.1 cm^{-1} are attributed mainly to C–H deformation and C–C stretching vibrations, respectively. The calculated frequency of 1429.1 cm^{-1} , with a relatively high IR intensity, shows good correspondence with the previously reported band near 1449 cm^{-1} . The calculated band at 1450.7 cm^{-1} also involves C–H deformation and related skeletal vibrations. A particularly important feature of the calculated spectrum is the presence of strong absorptions in the 1500–1800 cm^{-1} region. The band calculated at 1578.0 cm^{-1} is mainly associated with C=N and ring stretching vibrations and compares reasonably well with the previously reported value of approximately 1550 cm^{-1} . The calculated band at 1636.2 cm^{-1} can be assigned predominantly to C=O stretching and is in excellent agreement with the previously reported value of 1637 cm^{-1} . Two carbonyl stretching modes are calculated at 1721.2 and 1760.8 cm^{-1} . Although both modes contribute to the carbonyl stretching region, the difference between the calculated and previously reported values can be attributed to the harmonic approximation used in the theoretical calculations and to the differences between calculated gas-phase frequencies and experimental spectral conditions. The N–H stretching vibration is observed in the high-frequency region. The calculated band at 3642.9 cm^{-1} , with a relatively high IR intensity of 126.77 km mol^{-1} , is assigned to the N–H stretching mode and accounts for the prominent absorption observed around 3600 cm^{-1} in the calculated spectrum. In contrast, the calculated bands at 3122.7 and 3123.7 cm^{-1} are assigned to C–H stretching vibrations, rather than N–H stretching. These assignments are consistent with the normal-mode analysis of the optimized structure and provide a more reliable interpretation of the high-frequency region. The present vibrational analysis demonstrates satisfactory agreement with the previously reported FT-IR and DFT results. The most prominent calculated absorptions, particularly those associated with C=O, C–C, C–N, C=N, C–Cl, C–H, and N–H stretching vibrations, reproduce the characteristic spectral features of 8-chlorotheophylline. The calculated C=O stretching mode at 1636.2 cm^{-1} is in good agreement with the corresponding experimental and previously reported values, while the intense N–H stretching mode at 3642.9 cm^{-1} provides a reasonable assignment for the high-frequency absorption observed near 3600 cm^{-1} . The differences observed for some vibrational bands are expected because harmonic DFT frequencies may deviate from experimental values due to anharmonic effects and differences in the molecular environment. Thus, the vibrational frequency analysis provides further support for the reliability of the optimized 8-chlorotheophylline structure obtained at the B3LYP/6-311++G(d,p) level, providing a sound basis for the subsequent electronic-structure and nonlinear optical property analyses.

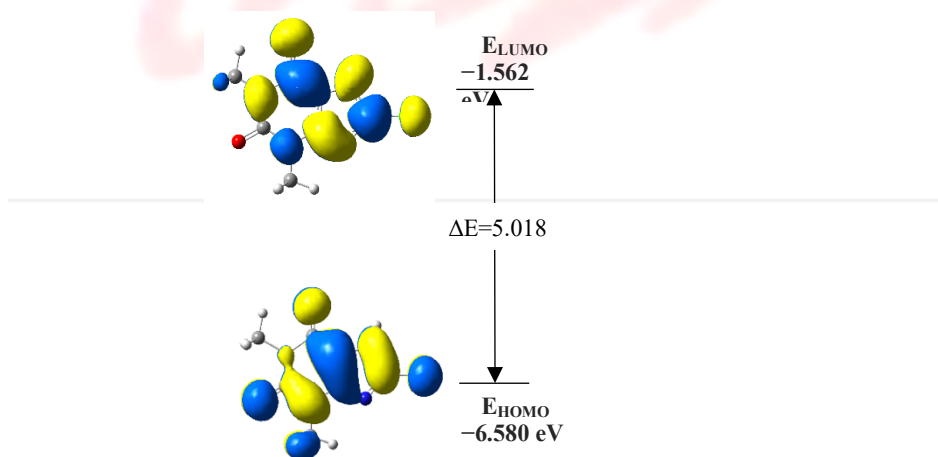
Table 2. Selected calculated vibrational frequencies, infrared intensities, and vibrational assignments of 8-chlorotheophylline in compared with literature data from Ref 10.

Calculated Frequency (cm ⁻¹)	Intensity (km mol ⁻¹)	Vibrational Assignment
3642.9	126.77	N–H stretching
3174.40	0.6426	C–H _{16,16,17} (asym) stretching
3167.28	0.4584	C–H _{19,20,21} (asym) stretching
3123.7	14.61	C–H _{15,17} (asym) stretching
3122.7	9.41	C–H _{20,21} (asym) stretching
3061.9	25.51	C–H _{15,16,17} (sym) stretching
3059.8	27.60	C–H _{19,20,21} (sym) stretching
1760.8	479.10	C=O₁₀, C=O₁₁, (sym) stretching
1721.2	926.68	C=O₁₀, C=O₁₁, (asym) stretching
1636.2	79.59	C1=C6 stretching
1578.0	107.83	C=N / ring stretching
1466.4	69.65	CH₃ wagging
1450.7	185.02	N–H rocking and C–H wagging
1445.6	24.83	C–N(Cl) stretching and CH₃ wagging
1429.1	364.96	C–N(Cl) stretching and CH₃ wagging
1401.7	80.23	Aromatic ring deformation and C=C stretching
1344.5	41.30	Aromatic ring deformation and N–CH ₃ bending
1288.9	38.93	Aromatic ring deformation and N–CH ₃ bending
1226.9	38.96	C–N / ring vibration
1120.4	28.46	C–N C–N rocking mode
1058.7	33.27	C–N stretching / ring vibration
988.4	50.60	Aromatic ring deformation and CH ₃ bending
752.5	25.23	Aromatic ring out-of-plane deformation
500.65	87.0714	N–H out-of-plane bending

Note: The most intense calculated IR bands are located at 1721.2, 1760.8, 1429.1, 1450.7, and 1578.0 cm⁻¹, corresponding predominantly to C=O stretching, C–C stretching, C–H deformation, and C=N/ring stretching vibrations, respectively. The calculated frequencies show good overall agreement with the reported literature (ref.10) values.

4. FRONTIER MOLECULAR ORBITAL (HOMO–LUMO) ANALYSIS

The frontier molecular orbital analysis was performed to investigate the electronic structure and chemical stability of 8-chlorotheophylline (CTP). The highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) were calculated for the optimized molecular geometry at the B3LYP/6-311++G(d,p) level using the Gaussian 09 program.

**Figure 3.** Frontier molecular orbitals (HOMO and LUMO) and their corresponding energy levels of CTP calculated at the B3LYP/6-311++G(d,p) level.

In the present study, the calculated HOMO energy is -6.580 eV, while the LUMO energy is -1.562 eV, giving a HOMO–LUMO energy gap of 5.018 eV is shown in Fig 3. The frontier molecular orbitals are mainly distributed over the conjugated xanthine ring system and the heteroatom-containing regions of the molecule. The HOMO represents the predominant electron-donating region, whereas the LUMO corresponds to the electron-accepting region. The spatial distributions of these orbitals therefore provide useful information about the possible intramolecular charge-transfer processes in CTP.

The HOMO–LUMO energy gap is an important parameter for evaluating the chemical stability and reactivity of a molecule. In general, a larger energy gap is associated with greater kinetic stability and lower chemical reactivity, whereas a smaller gap indicates that electronic excitation and charge transfer can occur more readily. The relatively large gap of 5.018 eV obtained in the present study therefore indicates a stable electronic structure for CTP.

The present results were compared with the previously reported DFT results of Prabavathi and Senthil Nayagi [10]. In the previous study, the HOMO and LUMO energies were reported as -7.7663 eV and -3.9972 eV, respectively, yielding a HOMO–LUMO gap of 3.7691 eV. In comparison, the present calculation gives HOMO and LUMO energies of -6.580 eV and -1.562 eV, respectively, with a corresponding energy gap of 5.018 eV. Thus, the present HOMO–LUMO gap is approximately 1.25 eV larger than the previously reported value.

The difference in the frontier orbital energies is noteworthy because both calculations employ the B3LYP/6-311++G(d,p) methodology. Such differences may originate from variations in the optimized molecular geometries, computational settings, or the electronic-density distribution obtained during the calculations. The difference is also reflected in the calculated dipole moment. The present study gives a dipole moment of 2.291727 D, whereas a value of 6.6032 D was reported in the previous study [10]. These differences indicate that the electronic properties of CTP are sensitive to the precise molecular geometry and electron distribution. Despite the numerical differences, both calculations predict a positive and relatively large HOMO–LUMO separation, supporting the conclusion that CTP possesses a comparatively stable electronic structure. The larger energy gap obtained in the present calculation suggests that the optimized structure considered in this study is less susceptible to low-energy electronic excitation than the structure reported previously.

Table 3. Frontier molecular orbital energies and HOMO–LUMO energy gaps of CTP obtained in the present and previous studies.

Parameter	Present study	Previous study [10]
HOMO (eV)	-6.5800	-7.7663
LUMO (eV)	-1.5620	-3.9972
HOMO–LUMO gap (eV)	5.0180	3.7691
Dipole moment (D)	2.2917	6.6032

Overall, the frontier molecular orbital analysis indicates that the present CTP structure has a relatively large HOMO–LUMO separation and consequently exhibits enhanced electronic stability. The differences between the present and previously reported frontier orbital energies emphasize the influence of molecular geometry and electron-density distribution on the calculated electronic properties.

6. ELECTRONIC ABSORPTION SPECTRUM (TD-DFT) ANALYSIS

The electronic absorption properties of 8-chlorotheophylline (CTP) were investigated using time-dependent density functional theory (TD-DFT) at the B3LYP/6-311++G(d,p) level. The calculated excitation energies, corresponding wavelengths, oscillator strengths (f), and dominant electronic transitions for the lowest singlet excited states are summarized in Table 4. As shown in Table 4 and Figure X, the lowest-energy transition, S1, occurs at 4.5942 eV (269.87 nm) and has the highest oscillator strength ($f = 0.1744$) among the calculated transitions. This strong absorption is predominantly associated with a HOMO→LUMO excitation and is assigned to a $\pi \rightarrow \pi^*$ transition. The relatively large oscillator strength indicates that S1 is an electronically allowed and intense transition, making it the most prominent feature of the calculated UV absorption spectrum.

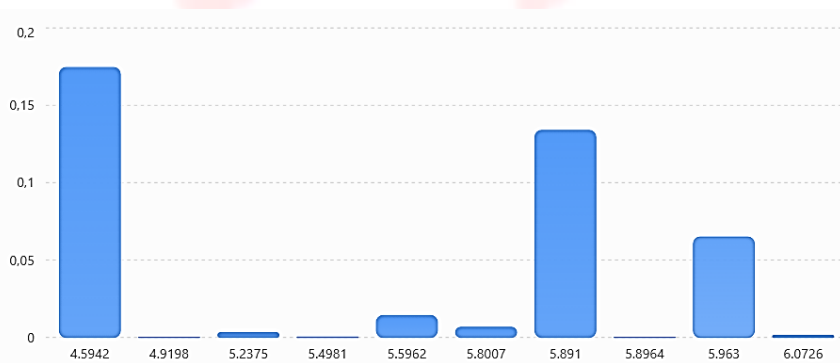


Figure 4. TD-DFT calculated electronic excitation spectrum, showing excitation energy (eV) on the x-axis and oscillator strength (f) on the y-axis.

The second major transition, S7, is located at 5.8910 eV (210.47 nm) with an oscillator strength of $f = 0.1338$. As evident from Table X and Figure X, this transition represents another strongly allowed electronic excitation in the high-energy region. Its contributions

involve more than one occupied and virtual orbital, indicating a more complex electronic character than that of S1. Nevertheless, the dominant contributions are consistent with a predominantly $\pi \rightarrow \pi^*$ excitation.

Another significant transition is S9, calculated at 5.9630 eV (207.92 nm) with $f = 0.0649$. This relatively high oscillator strength indicates a clearly allowed electronic transition and gives rise to an additional pronounced feature in the high-energy region of the calculated spectrum. The transition is assigned predominantly as $\pi \rightarrow \pi^*$ based on the character of the orbitals involved.

The transition S5, occurring at 5.5962 eV (221.55 nm) with $f = 0.0142$, has a considerably lower intensity than S1, S7, and S9. This excited state involves contributions from several orbital configurations and therefore exhibits a more mixed electronic character. Similarly, S6, calculated at 5.8007 eV (213.74 nm) with $f = 0.0066$, represents a weaker but identifiable electronic excitation and is predominantly associated with a $\pi \rightarrow \pi^*$ transition.

The remaining transitions, namely S2, S3, S4, S8, and S10, exhibit very low oscillator strengths ($f \leq 0.0030$) and are therefore expected to make only minor contributions to the overall absorption intensity. Although these transitions are included in Table X and Figure X, their weak oscillator strengths indicate that they are unlikely to produce prominent absorption features.

Overall, the TD-DFT results demonstrate that the calculated UV spectrum is dominated by three principal electronic transitions: S1 at 269.87 nm ($f = 0.1744$), S7 at 210.47 nm ($f = 0.1338$), and S9 at 207.92 nm ($f = 0.0649$). Among these, S1 corresponds to the lowest-energy and most intense excitation and is predominantly characterized as a HOMO $\rightarrow$ LUMO ($\pi \rightarrow \pi^*$) transition. The higher-energy transitions at approximately 210–208 nm further indicate the presence of strongly allowed π -electron excitations. The calculated spectrum therefore reflects the contribution of several π -electron transitions, with their relative intensities governed by the corresponding oscillator strengths.

Table 4. Calculated electronic excitation energies, wavelengths, oscillator strengths, and dominant molecular orbital contributions obtained from TD-DFT calculations at the B3LYP/6-311++G(d,p) level. The electronic transition assignments indicate the predominant character of the corresponding excited states.

State	λ (nm)	Energy (eV)	f	Main transition	Electronic transition assignment
S ₁	269.87	4.594	0.1744	HOMO $\rightarrow$ LUMO	$\pi \rightarrow \pi^*$
S ₂	252.01	4.920	0.0001	HOMO-1 $\rightarrow$ LUMO	$\pi \rightarrow \pi^*$
S ₃	236.73	5.238	0.0030	HOMO $\rightarrow$ LUMO+1	$\pi \rightarrow \pi^*$
S ₄	225.50	5.498	0.0002	HOMO $\rightarrow$ LUMO+2	$\pi \rightarrow \pi^*$
S ₅	221.55	5.596	0.0142	Mixed transitions	Karışık karakter; π katkısı önemli
S ₆	213.74	5.801	0.0066	HOMO $\rightarrow$ LUMO+3	$\pi \rightarrow \pi^*$
S ₇	210.47	5.891	0.1338	Mixed transitions	$\pi \rightarrow \pi^*$
S ₈	210.27	5.896	0.0001	HOMO-4 $\rightarrow$ LUMO	$\pi \rightarrow \pi^*$
S ₉	207.92	5.963	0.0649	Mixed transitions	$\pi \rightarrow \pi^*$
S ₁₀	204.17	6.073	0.0013	HOMO $\rightarrow$ LUMO+6	$\pi \rightarrow \pi^*$

The second singlet excited state (S₂), calculated at 252.01 nm, exhibits an oscillator strength close to zero ($f = 0.0001$), indicating that this transition is essentially symmetry-forbidden or only weakly allowed despite its relatively low excitation energy. Likewise, the S₃ and S₄ transitions possess very small oscillator strengths, suggesting negligible contributions to the absorption spectrum.

More intense electronic transitions are predicted at higher energies. In particular, the S₇ state at 210.47 nm exhibits a relatively large oscillator strength ($f = 0.1338$), while the S₉ state at 207.92 nm also contributes significantly with an oscillator strength of 0.0649. Unlike the S₁ excitation, these higher-energy absorptions arise from mixed electronic configurations involving several occupied and virtual molecular orbitals, reflecting a more complex redistribution of electron density upon excitation.

Comparison of the TD-DFT results with the frontier molecular orbital analysis indicates that the lowest-energy absorption band is governed primarily by the HOMO–LUMO excitation, whereas the higher-energy bands involve transitions from deeper occupied orbitals to higher virtual orbitals. This behavior is consistent with the electronic structure of the molecule and confirms that the frontier molecular orbitals play a dominant role in determining the optical properties of 8-chlorotheophylline.

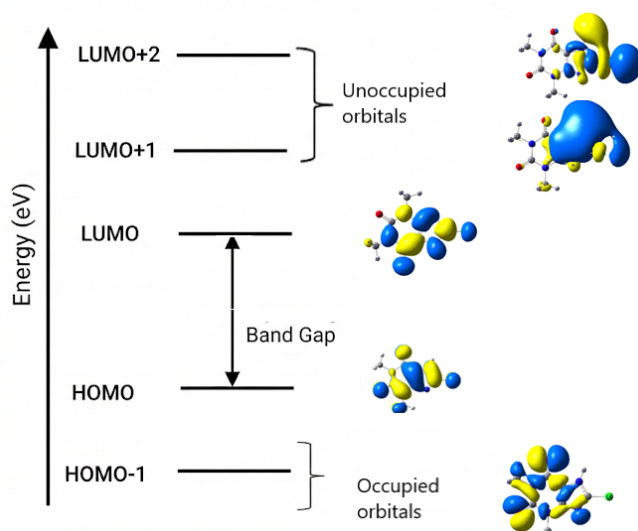


Figure 5. Molecular orbital plots of the HOMO–1, HOMO, LUMO, LUMO+1, and LUMO+2 orbitals of CTP calculated at the B3LYP/6-311++G(d,p) level.

The calculated molecular orbitals provide insight into the electronic structure and possible electronic transitions of CTP, as shown in Figure 5. The occupied orbitals (HOMO–1 and HOMO) and unoccupied orbitals (LUMO, LUMO+1, and LUMO+2) exhibit distinct spatial distributions over the molecular framework, reflecting their different electronic characters. These orbital distributions form the basis for the assignment and interpretation of the electronic transitions obtained from the TD-DFT calculations.

Overall, the TD-DFT calculations predict that the electronic absorption spectrum of CTP is characterized by one prominent absorption band around 270 nm, accompanied by additional weaker and higher-energy transitions in the 200–220 nm region. These findings provide valuable insight into the excited-state electronic structure of the molecule and complement the HOMO–LUMO analysis presented in the previous section.

5. MOLECULAR ELECTROSTATIC POTENTIAL (MEP) ANALYSIS

The molecular electrostatic potential (MEP) surface was calculated to identify the electrophilic and nucleophilic reactive sites of 8-chlorotheophylline. The MEP surface mapped onto the electron density is presented in Fig. 5. The color scale ranges from red (most negative electrostatic potential) to blue (most positive electrostatic potential), with green representing regions of nearly neutral potential. As illustrated in Fig. 5, the negative electrostatic potential is mainly localized around the oxygen atoms, indicating favorable sites for electrophilic attack. In contrast, the positive electrostatic potential is concentrated around the hydrogen atoms, suggesting preferred regions for nucleophilic attack. The remaining parts of the molecule exhibit intermediate electrostatic potential values, reflecting a relatively balanced charge distribution over the molecular surface.

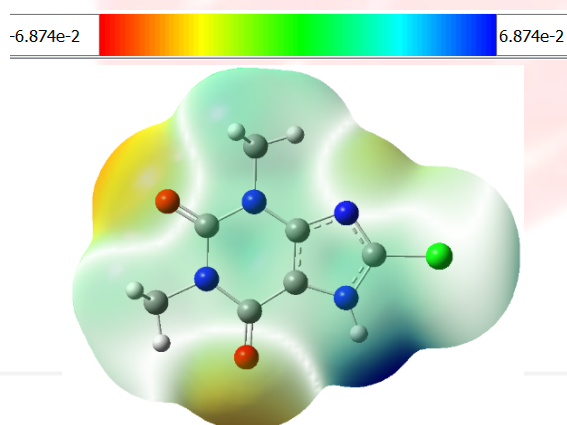


Figure 5. Molecular electrostatic potential (MEP) surface of 8-chlorotheophylline calculated at the B3LYP/6-311++G(d,p) level of theory. The color scale ranges from red (most negative electrostatic potential) to blue (most positive electrostatic potential).

7. DISCUSSION

The structural, vibrational, and electronic properties of 8-chlorotheophylline (CTP) were investigated using density functional theory at the B3LYP/6-311++G(d,p) level. The calculations were performed with the Gaussian 09 program. The combined analysis of the optimized molecular geometry, vibrational frequencies, dipole moment, and frontier molecular orbitals provides a consistent description of the structural stability and electronic characteristics of the molecule.

The geometry optimization yielded a stable molecular structure with a total electronic energy of -1100.847 Hartree. The optimized C8–C12 bond length of 1.7171 Å reflects the characteristic bonding environment of the optimized structure. Importantly, the subsequent vibrational analysis revealed no imaginary frequencies, confirming that the optimized geometry corresponds to a true

minimum on the potential energy surface. This provides a reliable structural basis for the subsequent electronic and vibrational analyses.

The calculated vibrational spectrum reproduces the characteristic spectral features of CTP. The most significant calculated bands are associated with C–Cl, C–N, C–C, C=N, C=O, C–H, and N–H vibrational motions. Particularly good agreement with the previously reported results is obtained for the C=O stretching vibration at 1636.2 cm^{-1} , compared with the previously reported value of approximately 1637 cm^{-1} . In the high-frequency region, the calculated bands at 3122.7 and 3123.7 cm^{-1} are assigned to C–H stretching vibrations, whereas the intense band at 3642.9 cm^{-1} is attributed to the N–H stretching vibration and accounts for the prominent high-frequency absorption observed around 3600 cm^{-1} . These assignments are consistent with the corresponding normal-mode analyses. The good agreement observed for the characteristic C=O and N–H stretching regions supports the reliability of the optimized molecular structure and the computational methodology employed in the present study. Some differences between the calculated and previously reported vibrational frequencies are observed, particularly for the carbonyl and skeletal stretching modes. Such differences are expected because the calculated values correspond to harmonic frequencies for an isolated molecule, whereas experimental vibrational spectra are affected by anharmonicity, intermolecular interactions, and experimental conditions. Nevertheless, the overall correspondence between the calculated and previously reported bands demonstrates that the main vibrational characteristics of CTP are successfully reproduced.

The calculated dipole moment of 2.291727 D indicates a non-symmetric distribution of electronic charge within the molecule. The presence of several electronegative O, N, and Cl atoms contributes significantly to this charge distribution. The dipole moment obtained in the present study is lower than the previously reported value of 6.6032 D [10]. This difference, together with the differences observed in the frontier molecular orbital energies, suggests that the precise optimized geometry and resulting electron-density distribution have a significant influence on the calculated electronic properties of CTP.

The HOMO–LUMO analysis provides further insight into the electronic stability of the molecule. In the present calculation, the HOMO and LUMO energies were determined to be -6.5800 eV and -1.5620 eV , respectively, resulting in a HOMO–LUMO energy gap of 5.0180 eV . In comparison, the previously reported values were -7.7663 eV for the HOMO and -3.9972 eV for the LUMO, corresponding to a gap of 3.7691 eV [10].

The HOMO–LUMO gap obtained in the present study is therefore approximately 1.25 eV larger than the previously reported value. A larger energy gap is generally associated with enhanced kinetic stability and reduced chemical reactivity because a greater amount of energy is required for electronic excitation from the occupied to the unoccupied molecular orbital. Consequently, the present calculation suggests that the optimized CTP structure possesses comparatively high electronic stability.

The difference between the present and previous HOMO–LUMO results is particularly interesting because both studies employ the B3LYP/6-311++G(d,p) methodology. Therefore, the observed differences are likely related to the specific optimized geometry and the corresponding electron-density distribution rather than simply to the choice of functional or basis set. The simultaneous differences in the calculated dipole moments support this interpretation. Thus, the present results emphasize the importance of using the actual optimized molecular structure when evaluating the electronic properties of CTP.

Taken together, the optimized geometry, vibrational spectrum, dipole moment, frontier molecular orbital analysis, and molecular electrostatic potential provide mutually consistent evidence for the stability and electronic characteristics of the calculated CTP structure. The absence of imaginary frequencies confirms that the optimized geometry corresponds to a true minimum on the potential energy surface, while the relatively large HOMO–LUMO energy gap indicates considerable electronic stability. The MEP analysis identifies the oxygen atoms as the most electron-rich regions and the hydrogen atoms as the most electron-deficient regions, revealing the preferred sites for electrophilic and nucleophilic interactions. Furthermore, the satisfactory agreement of the characteristic vibrational bands with the previous study supports the reliability of the present calculations. At the same time, the differences observed in the dipole moment and frontier orbital energies demonstrate that the electronic properties of CTP are sensitive to the precise molecular geometry and the resulting electron-density distribution.

In addition to the ground-state electronic properties, the excited-state behavior of 8-chlorotheophylline was investigated using time-dependent density functional theory (TD-DFT) at the same level of theory. The calculated singlet excitation energies and oscillator strengths indicate that the first optically allowed electronic transition occurs at 269.87 nm (4.5942 eV) with an oscillator strength of 0.1744 , arising predominantly from the HOMO $\rightarrow$ LUMO transition (Table 4). This result demonstrates that the lowest-energy absorption band is mainly governed by the frontier molecular orbitals identified in the ground-state calculations. Several additional singlet excited states were predicted in the $204\text{--}252\text{ nm}$ region. However, most of these transitions exhibit very small oscillator strengths, indicating weak contributions to the electronic absorption spectrum. More intense absorption bands were calculated at 210.47 nm ($f = 0.1338$) and 207.92 nm ($f = 0.0649$), which originate from mixed electronic excitations involving multiple occupied and virtual molecular orbitals. The TD-DFT results therefore suggest that the electronic absorption spectrum of CTP is characterized by one dominant low-energy absorption band near 270 nm , together with several higher-energy transitions in the ultraviolet region. The agreement between the frontier molecular orbital analysis and the TD-DFT calculations confirms that the optical properties of CTP are strongly influenced by the electronic distribution of the highest occupied and lowest unoccupied molecular orbitals, while higher-energy absorptions arise from more complex orbital interactions.

Overall, the present DFT and TD-DFT results provide a coherent theoretical description of the structural, vibrational, electronic, electrostatic, and excited-state properties of 8-chlorotheophylline. The optimized molecular geometry, confirmed by the absence of

imaginary frequencies, provides a reliable basis for the calculated molecular properties. The vibrational analysis reproduces the characteristic spectral features reported in the literature, supporting the validity of the computational methodology. The relatively large HOMO–LUMO energy gap indicates considerable electronic stability, whereas the MEP analysis identifies the oxygen atoms as the most electron-rich regions and the hydrogen atoms as the most electron-deficient sites, indicating the preferred locations for electrophilic and nucleophilic interactions. Furthermore, the TD-DFT calculations reveal that the lowest-energy electronic absorption is dominated by the HOMO → LUMO excitation, while higher-energy absorptions arise from mixed orbital transitions. Collectively, these findings provide a comprehensive theoretical understanding of the structural and electronic behavior of CTP and establish a solid foundation for future investigations of its photophysical, photochemical, and nonlinear optical properties.

8.CONCLUSION

In this study, the structural, vibrational, electronic, and excited-state properties of 8-chlorotheophylline (CTP) were systematically investigated using DFT and TD-DFT calculations at the B3LYP/6-311++G(d,p) level. The optimized molecular geometry was confirmed to correspond to a true minimum on the potential energy surface by the absence of imaginary vibrational frequencies. The calculated vibrational frequencies and their assignments successfully reproduced the characteristic vibrational features of CTP and showed good agreement with the available literature data, supporting the reliability of the computational methodology.

The frontier molecular orbital analysis revealed a HOMO–LUMO energy gap of 5.0180 eV, indicating considerable electronic stability of the molecule. Furthermore, the molecular electrostatic potential analysis identified the oxygen atoms as the most electron-rich regions and the hydrogen atoms as the most electron-deficient sites, providing insight into the possible reactive regions of the molecule.

The TD-DFT calculations provided valuable information on the electronic excitation properties of CTP. The first allowed electronic transition was predicted at 269.87 nm and was found to be dominated by the HOMO → LUMO excitation, while the higher-energy absorption bands originated from mixed orbital transitions involving several occupied and virtual molecular orbitals. These results demonstrate that the optical response of CTP is closely related to its frontier electronic structure.

Overall, the present theoretical investigation provides a comprehensive understanding of the structural, vibrational, electronic, electrostatic, and excited-state properties of 8-chlorotheophylline. The combined DFT and TD-DFT results establish a reliable theoretical foundation for future experimental studies and for further investigations of the photophysical, photochemical, and nonlinear optical properties of this molecule.

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F-6

PHOTOISOMERIZATION and CONFORMATIONAL ANALYSIS of MATRIX-ISOLATED PHTHALIC ACID

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ABSTRACT

The conformational landscape of phthalic acid (PA) isolated in solid argon at 15 K was investigated by matrix-isolation Fourier-transform infrared (FTIR) spectroscopy in combination with density functional theory (DFT) calculations. The conformational stability, optimized geometries, and vibrational spectra of the low-energy conformers were evaluated at the B3LYP/6-311++G(d,p) level. Three stable conformers, PA₁, PA₂, and PA₃, were identified, with PA₁ predicted to be the global minimum and PA₂ and PA₃ lying 0.70 and 2.85 kJ mol⁻¹ above PA₁, respectively. Comparison of the calculated vibrational frequencies and infrared intensities with the experimental matrix-isolation spectrum enabled the characteristic bands of the three conformers to be assigned. The O–H stretching region provides the clearest spectroscopic evidence for conformer coexistence, with the dominant band at 3563.1 cm⁻¹ assigned mainly to PA₂, the shoulder near 3565–3566 cm⁻¹ associated with PA₃, and the feature near 3571.1 cm⁻¹ attributed to the free O–H stretching modes of PA₁ and PA₂. Additional agreement in the C=O, C–O, and aromatic ring vibrational regions further supports the simultaneous presence of all three conformers in the argon matrix. The combined experimental and theoretical results provide a consistent description of the conformational composition and vibrational behavior of matrix-isolated phthalic acid.

Keywords: Matrix-isolation FTIR spectroscopy; Phthalic acid; Density functional theory (DFT); Conformational analysis; Vibrational spectroscopy.

1. INTRODUCTION

Phthalic acid (benzene-1,2-dicarboxylic acid, PA) is one of the simplest aromatic dicarboxylic acids and has long served as a model system for investigating the structural, vibrational, and photochemical properties of molecules containing adjacent carboxyl groups [1]. Besides its fundamental importance in physical chemistry, phthalic acid and its derivatives are extensively employed as intermediates in the production of polymers, pharmaceuticals, dyes, and functional organic materials [2]. Owing to the presence of two neighboring carboxyl groups, PA exhibits pronounced conformational flexibility arising from rotation about the C–C bonds and the formation of intramolecular hydrogen-bonding interactions. Consequently, several conformers with small relative energy differences may coexist, making this molecule an attractive prototype for studying conformational equilibria and photoinduced structural transformations [3].

The experimental characterization of isolated conformers is often hindered by intermolecular interactions in the condensed phase, where hydrogen bonding, crystal packing, or molecular aggregation considerably broaden and distort vibrational spectra. Matrix-isolation spectroscopy overcomes these limitations by trapping isolated molecules in an inert rare-gas matrix at cryogenic temperatures, effectively suppressing intermolecular interactions while preserving individual conformers and reactive intermediates [4]. Combined with high-resolution Fourier-transform infrared (FTIR) spectroscopy and quantum-chemical calculations, this technique provides an exceptionally powerful approach for identifying molecular structures, assigning vibrational bands, and investigating conformational dynamics under well-controlled conditions [4–6].

Over the past decades, matrix-isolation spectroscopy has been extensively employed to investigate conformational isomerism and structural transformations in carboxylic acids. These studies have demonstrated that cryogenic matrix isolation, combined with infrared spectroscopy and quantum-chemical calculations, provides an effective approach for identifying individual conformers and elucidating their structural and vibrational characteristics [5–13]. A number of representative examples illustrate the versatility of this approach. Rotational isomerism and UV-induced conformational conversion have been thoroughly investigated for acrylic acid, where matrix-isolation experiments combined with *ab initio* calculations enabled the identification of individual conformers and the elucidation of their photochemical interconversion mechanisms [7,8]. Similar studies on chloroacetic acid, crotonic acid, pyruvic acid, fumaric acid, and maleic acid revealed the formation of higher-energy conformers following selective vibrational excitation, providing detailed information on potential-energy surfaces, intramolecular hydrogen-bond rearrangements, and vibrational energy redistribution [5,9–11]. More recently, narrow-band near-infrared excitation has been shown to constitute an efficient and highly selective tool for inducing conformational switching through excitation of OH-stretching overtone vibrations, allowing direct experimental observation of conformers that are not thermally populated under equilibrium conditions [11].

Previous studies have demonstrated that matrix-isolated carboxylic acids can undergo efficient conformational switching, photorotamerization, and isomerization upon near-infrared (NIR) and ultraviolet (UV) irradiation, providing valuable insights into the mechanisms governing conformational interconversion in cryogenic matrices [11–14]. An early comprehensive vibrational study of *o*-phthalic acid by Colombo et al. combined infrared and Raman spectroscopy with normal coordinate analysis, providing detailed assignments of its fundamental vibrational modes [15]. These results provide an important reference for the interpretation of the vibrational spectra of phthalic acid and its conformers. Loring et al. investigated the infrared spectra of phthalic acid, hydrogen phthalate, and phthalate in aqueous solution at different pH values, assigning their characteristic vibrational bands through factor analysis and *ab initio* calculations [16]. Their results provide useful reference data for the interpretation of the characteristic carboxylic acid and carboxylate vibrations of phthalic acid.

In the present work, we investigate the conformational behavior and photoinduced transformations of matrix-isolated phthalic acid, with particular emphasis on the effects of NIR irradiation on its conformational equilibria.

Despite the extensive body of work devoted to aliphatic carboxylic acids and several substituted aromatic systems, comparatively little attention has been paid to the conformational dynamics and photoinduced behavior of phthalic acid. Although its equilibrium molecular structure and vibrational spectra have been reported, a comprehensive matrix-isolation investigation combining experimental infrared spectroscopy with density functional theory (DFT) calculations and selective near-infrared-induced conformational interconversion has remained unavailable. Considering the unique structural characteristics of PA, particularly the competition between intramolecular hydrogen bonding and steric interactions associated with adjacent carboxyl groups, such a study is expected to provide valuable insight into the mechanisms governing conformational stability and photoisomerization in aromatic dicarboxylic acids.

In the present work, the conformational landscape and photoinduced behavior of phthalic acid isolated in solid argon at 15 K were investigated by matrix-isolation FTIR spectroscopy supported by DFT calculations performed at the B3LYP/6-311++G(d,p) level. The calculated equilibrium geometries, relative conformational energies, and harmonic vibrational frequencies were employed to identify the experimentally observed conformers and assign the infrared spectra. Furthermore, selective near-infrared irradiation was used to induce conformational interconversion between the low-energy conformers, providing direct insight into the structural dynamics and photoisomerization pathways of phthalic acid under isolated cryogenic conditions.

2. THEORETICAL CALCULATION

Theoretical calculations were performed using the Gaussian 09 program package. The molecular geometries of the relevant phthalic acid conformers were fully optimized at the B3LYP/6-311++G(d,p) level of theory, where B3LYP denotes the Becke three-parameter hybrid exchange functional combined with the Lee–Yang–Parr correlation functional [17, 18]. Harmonic vibrational frequency calculations were subsequently performed at the same level to characterize the optimized structures as minima on the potential-energy surface and to obtain the corresponding infrared frequencies and intensities. The relative conformational energies were calculated from the optimized structures, and the resulting energy ordering was used to identify the experimentally observed conformers. The calculated vibrational frequencies and infrared intensities were compared with the experimental matrix-isolation FTIR spectra to assist in the assignment of the observed absorption bands. This computational approach is consistent with the methodology commonly employed in matrix-isolation studies of conformational isomerism.

3. CONFORMATIONAL ANALYSIS

Phthalic acid (PA), an aromatic dicarboxylic acid, possesses two adjacent carboxyl groups attached to a benzene ring, giving rise to considerable conformational flexibility. The optimized molecular structure together with the atom numbering used throughout this work is shown in Figure 1. This numbering scheme is employed for the assignment of geometrical parameters and vibrational modes discussed in the following sections.

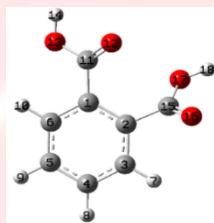


Figure 1. Optimized molecular structure and atom numbering of phthalic acid calculated at the B3LYP/6-311++G(d,p) level.

Phthalic acid (PA) exhibits considerable conformational flexibility due to internal rotation of its two carboxylic acid groups about the C–C bonds connecting them to the benzene ring. Variations in the orientation of the hydroxyl groups give rise to several energetically accessible conformations, each characterized by distinct intramolecular interactions and hydrogen-bonding patterns. In the present study, a systematic conformational search followed by geometry optimization at the B3LYP/6-311++G(d,p) level located three stable minima on the potential energy surface, denoted as PA₁, PA₂, and PA₃. The optimized molecular structures are presented in Figure 2.

The three conformers differ primarily in the relative orientation of the two carboxylic acid groups. PA₁ adopts a mixed cis/trans arrangement, PA₂ corresponds to the cis/cis configuration, whereas PA₃ possesses a trans/trans orientation. These structural differences influence the extent of intramolecular O–H···O interactions, steric repulsion between adjacent substituents, and the degree of π -conjugation between the carboxyl groups and the aromatic ring, thereby determining the relative stability of each conformer.

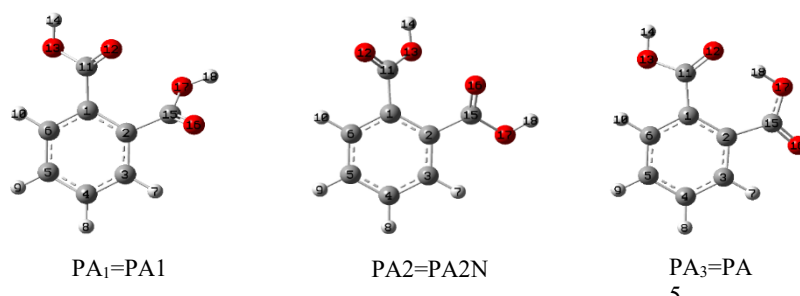


Figure 2. Optimized molecular geometries of the three stable conformers of phthalic acid (PA₁, PA₂ and PA₃) calculated at the B3LYP/6-311++G(d,p) level. The conformers differ in the relative orientation of the two carboxylic acid groups, corresponding to cis/trans (PA₁), cis/cis (PA₂), and trans/trans (PA₃) arrangements.

The calculated relative electronic energies are summarized in Table 1. PA₁ is predicted to be the global minimum on the potential energy surface. The PA₂ conformer is only 0.70 kJ mol⁻¹ (with ZPVE) higher in energy, while PA₃ lies 2.85 kJ mol⁻¹ (with ZPVE) above the global minimum. These very small energy differences indicate a shallow potential energy surface and demonstrate the pronounced conformational flexibility of phthalic acid. Such small energy separations suggest that more than one conformer may be populated under experimental conditions, particularly prior to matrix isolation.

Table 1. Relative electronic energies and conformational assignments of the optimized phthalic acid conformers.

Conformer	ΔE (kJ mol ⁻¹)	Carboxyl-group orientation
PA ₁	0.00	cis / trans
PA ₂	0.70	cis / cis
PA ₃	2.85	trans / trans

The conformational preferences obtained in the present work are in excellent agreement with the comprehensive conformational analysis of benzenedicarboxylic acids reported by Marković, Badjuk, and Gutman using semiempirical AM1 calculations [19]. Their study identified three symmetry-distinct minima for phthalic acid, corresponding to the mixed cis/trans, cis/cis, and trans/trans arrangements of the two carboxylic acid groups.

The same three conformers (PA₁–PA₃) were located in the present investigation using the B3LYP/6-311++G(d,p) method, and the predicted energetic ordering is identical, with the cis/trans conformer representing the global minimum. This excellent agreement demonstrates that the intrinsic conformational preferences of phthalic acid are largely independent of the theoretical approach and are primarily governed by intramolecular steric and electronic interactions.

Compared with the earlier AM1 investigation, the present study provides a substantially more reliable and quantitative description of the potential energy surface through the use of hybrid density functional theory together with a triple- ζ basis set including diffuse and polarization functions. While the AM1 calculations successfully reproduced the overall topology of the conformational landscape, the present DFT calculations yield more accurate relative energies and optimized molecular geometries. Moreover, the present work extends the previous theoretical study by providing harmonic vibrational frequencies, infrared intensities, and normal-mode assignments, which enable direct correlation with the experimental matrix-isolation FTIR spectra. The calculated energy differences between PA₁, PA₂, and PA₃ (0.00, 0.70, and 2.85 kJ mol⁻¹, respectively) further confirm the shallow conformational potential energy surface proposed by Marković et al., while offering a quantitatively more reliable energetic description. Consequently, the present investigation not only confirms the conformational model proposed in the earlier semiempirical study but also provides a comprehensive structural and spectroscopic characterization of phthalic acid based on modern DFT calculations and experimental validation.

As shown in Fig. 3, the simulated spectra illustrate the characteristic vibrational features of each conformer and provide a direct comparison of their relative spectral patterns, facilitating the assignment of the experimental bands observed for phthalic acid isolated in an argon matrix at 15 K.

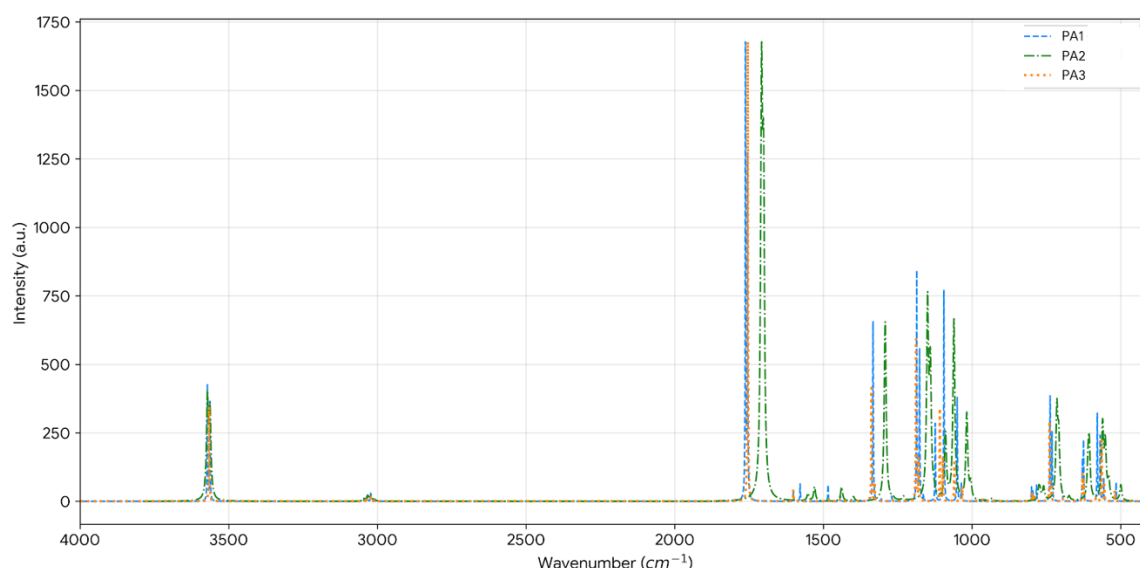


Figure 3. Calculated infrared spectra of the three phthalic acid conformers, scaled by a factor of 0.948, PA₁, PA₂, and PA₃, obtained at the B3LYP/6-311++G(d,p) level of theory. The simulated spectra illustrate the characteristic vibrational features of each conformer and provide a direct comparison of their relative spectral patterns, facilitating the assignment of the experimental bands observed for phthalic acid isolated in an argon matrix at 15 K.

4. COMPARISON of EXPERIMENTAL and THEORETICAL RESULTS

Phthalic acid was isolated in a solid argon matrix at 15 K using a conventional matrix-isolation technique. The sample was vaporized under controlled heating and co-deposited with high-purity argon onto a precooled CsI window mounted in a closed-cycle helium cryostat. Infrared spectra were recorded in the 4000–400 cm^{-1} region using an FTIR spectrometer. The matrix temperature and deposition conditions were optimized to favor the isolation of monomeric phthalic acid and to minimize aggregation. Phthalic acid (PA), an aromatic dicarboxylic acid, possesses two adjacent carboxyl groups attached to a benzene ring, giving rise to considerable conformational flexibility.

For comparison with the experimental FTIR spectrum, the harmonic vibrational frequencies calculated at the B3LYP/6-311++G(d,p) level were scaled by a factor of 0.948. The value of 0.948 was determined empirically in the present study based on the systematic frequency shift between the calculated and experimental bands. This factor provided the best overall correspondence with the experimental spectrum obtained under argon matrix-isolation conditions.

O–H Stretching Region: 3600–3500 cm^{-1}

The high-frequency region of the matrix-isolation FTIR spectrum, between 3600 and 3500 cm^{-1} , provides particularly important evidence for the coexistence of different phthalic acid conformers in the argon matrix (Fig. 4). The experimental spectrum exhibits several distinct features centered at approximately 3571.1, 3563.1, and 3557.4 cm^{-1} , rather than a single isolated O–H stretching band. The overall spectral structure is reproduced by the calculated vibrational signatures of PA₁, PA₂, and PA₃.

The calculated spectrum of PA₁ shows O–H stretching bands at 3571.3 and 3562.5 cm^{-1} , whereas PA₂ exhibits corresponding bands at 3570.9 and 3562.7 cm^{-1} . The calculated bands near 3571 cm^{-1} for both PA₁ and PA₂ are in excellent agreement with the experimental feature at 3571.1 cm^{-1} . These bands are associated with the stretching vibration of the relatively weakly perturbed, or free, O–H group. The close correspondence indicates that both PA₁ and PA₂ contribute to the experimental feature in this region. The most intense experimental band at 3563.1 cm^{-1} is in excellent agreement with the calculated O–H stretching vibration of PA₂ at 3562.7 cm^{-1} . This correspondence, together with the relatively high calculated intensity of this mode, indicates that PA₂ provides the dominant contribution to the experimental band at 3563.1 cm^{-1} . The calculated O–H stretching vibration of PA₃ at 3565.7 cm^{-1} lies on the higher-frequency side of this experimental feature and is therefore consistent with a contribution to the corresponding shoulder or broadened spectral envelope. The lower-frequency experimental contribution extending toward approximately 3557 cm^{-1} is also associated with the broadened hydrogen-bonded O–H stretching envelope associated primarily with PA₂.

Thus, the experimental O–H stretching profile is best interpreted as the combined contribution of the three conformers, with PA₂ making the dominant contribution around 3563 cm^{-1} , PA₃ contributing to the higher-frequency side of this band, and PA₁ and PA₂ contributing to the free O–H stretching feature near 3571 cm^{-1} . The simultaneous correspondence of these experimental features with the calculated vibrational signatures provides strong spectroscopic evidence for the coexistence of PA₁, PA₂, and PA₃ in the argon matrix.

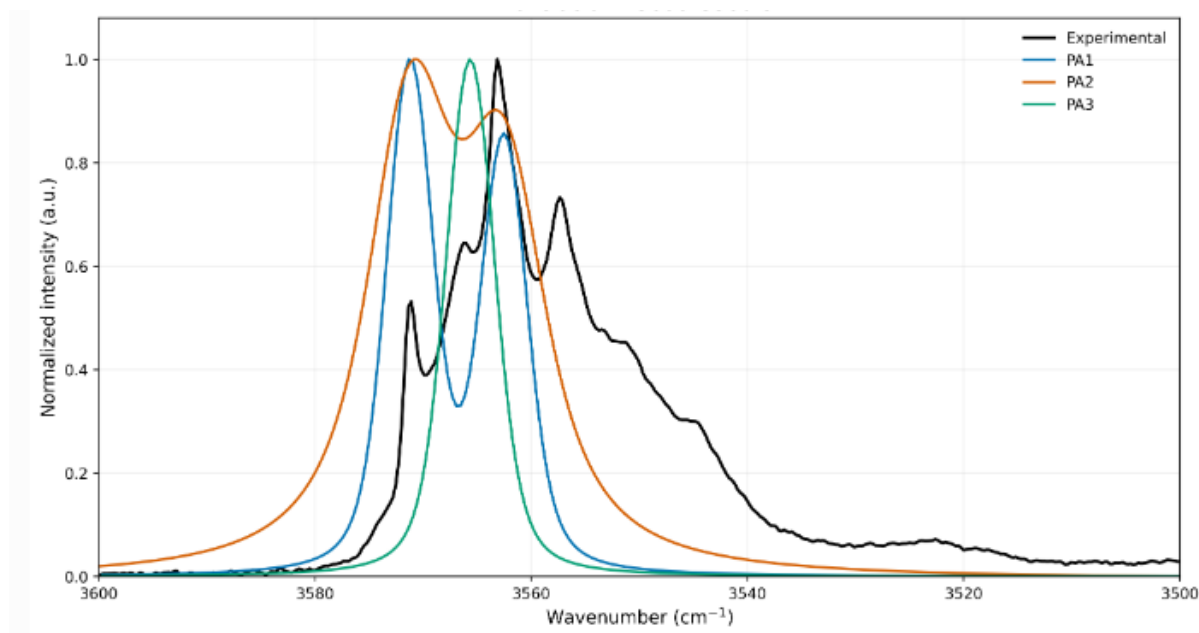


Figure 4. Experimental and calculated infrared spectra of phthalic acid (PA) isolated in an argon matrix at 15 K, focusing on the O–H stretching region (3600–3500 cm^{-1}). The calculated spectra correspond to the PA₁, PA₂, and PA₃ conformers obtained at the B3LYP/6-311++G(d,p) level of theory.

The calculated spectra were broadened using a FWHM of 4 cm^{-1} , and the intensities of the experimental and calculated spectra were independently scaled for visualization within the plotted spectral region. Therefore, the relative peak heights in the figure are intended to facilitate comparison of the vibrational band positions and spectral patterns and should not be interpreted as quantitative experimental-to-theoretical intensity ratios. Importantly, the frequency agreement and the overall band pattern, rather than the absolute intensities, provide the basis for the conformer assignments.

The excellent correspondence between the experimental O–H stretching features and the calculated vibrational signatures of PA₁, PA₂, and PA₃ provides strong evidence that the three conformers are simultaneously present in the argon matrix. The observation of multiple O–H stretching signatures within this narrow spectral region therefore constitutes one of the clearest spectroscopic indications of conformer coexistence under the matrix-isolation conditions.

The experimental spectrum in the O–H stretching region exhibits several distinct features between 3575 and 3560 cm^{-1} . The prominent band near 3563 cm^{-1} is consistent with the intramolecularly hydrogen-bonded O–H stretching modes of PA₁ and PA₂, calculated at 3562.5 and 3562.7 cm^{-1} , respectively. A higher-frequency shoulder near 3566 cm^{-1} is assigned to the intramolecularly hydrogen-bonded O–H stretching mode of PA₃, calculated at 3565.7 cm^{-1} . The feature near 3571 cm^{-1} is attributed to the free O–H stretching modes of PA₁ and PA₂. These assignments are consistent with the calculated vibrational frequencies and the simulated spectra of the three conformers.

Additional experimental features at 1767–1773 cm^{-1} and around 1103 cm^{-1} are also consistent with contributions from PA₁, as summarized in Table 2. In particular, PA₂ is characterized by a strong intramolecular O–H $\cdots$ O hydrogen bond, which significantly affects its carbonyl stretching vibration and gives rise to calculated hydrogen-bonded C=O stretching modes at approximately 1707.5 and 1702.0 cm^{-1} . These low-frequency C=O stretching modes provide important spectroscopic signatures of the hydrogen-bonded PA₂ conformer, consistent with the experimental feature observed near 1713 cm^{-1} .

Comparison of Calculated and Experimental Vibrational Spectra in the 1900–800 cm^{-1} region

A detailed comparison of the experimental and calculated infrared spectra in the 1900–800 cm^{-1} region reveals a close correspondence between the observed bands and the characteristic vibrational modes predicted for PA₁, PA₂, and PA₃ (Fig. 5, Table 2). The assignments indicate that the experimental spectrum is not adequately represented by a single conformer, but instead contains contributions from all three conformational structures.

The most diagnostic region is that of the carbonyl stretching vibrations. PA₁ exhibits two calculated C=O stretching modes at 1762.1 and 1754.9 cm^{-1} , while PA₃ has a corresponding mode at 1754.1 cm^{-1} . The experimental feature at 1759.0 cm^{-1} is in close agreement with these calculated modes, indicating overlapping contributions from PA₁ and PA₃. The additional experimental components observed in the 1767–1773 cm^{-1} region are not directly reproduced by the calculated fundamental frequencies. In contrast, PA₂ displays characteristic hydrogen-bonded C=O stretching modes at 1707.5 and 1702.0 cm^{-1} , which can be associated with the experimental band at 1713.0 cm^{-1} . The clear separation of the PA₂ carbonyl stretching modes from those of PA₁ and PA₃ provides a useful spectroscopic distinction between the conformers.

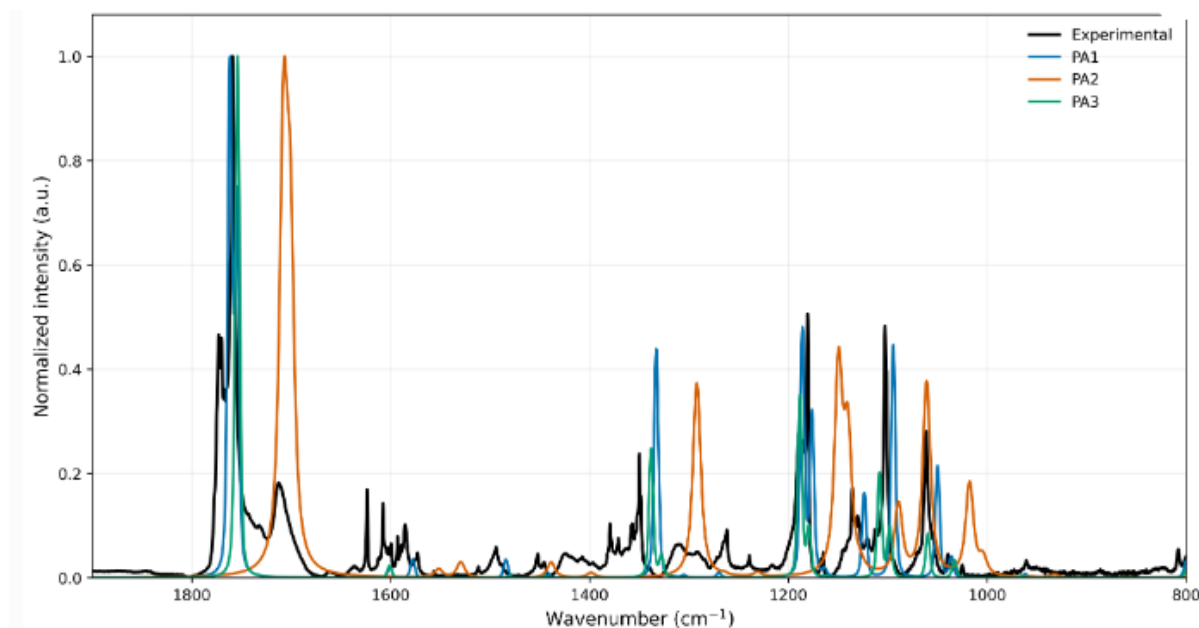


Figure 5. Experimental and calculated infrared spectra of PA (scaled by a factor of 0.948) isolated in an argon matrix at 15 K, covering the 1900–800 cm^{-1} spectral region. The calculated spectra correspond to the PA₁, PA₂, and PA₃ conformers obtained at the B3LYP/6-311++G(d,p) level of theory.

The region between approximately 1650 and 1500 cm^{-1} is dominated by vibrational modes involving the aromatic ring. The calculated feature of PA₃ at 1601 cm^{-1} and the corresponding ring stretching contribution in PA₁ are associated with the experimental band at 1608 cm^{-1} . The additional experimental features at 1593 and 1585 cm^{-1} , together with the band at 1573 cm^{-1} , can be attributed to combinations of aromatic C=C stretching and ring deformation modes. In particular, the calculated PA₁ mode at 1578 cm^{-1} provides a reasonable correspondence with the experimental structure in this region. The experimental band at 1624 cm^{-1} is weaker and is most appropriately considered as a coupled aromatic ring deformation/stretching feature rather than as a distinct conformer-specific band.

Between 1500 and 1400 cm^{-1} , the calculated modes are predominantly associated with aromatic C–C stretching, C–H bending, and ring deformation. The PA₁ mode at 1484 cm^{-1} is consistent with the experimental feature near 1494 cm^{-1} , while the calculated PA₁ and PA₂ modes at 1443 and 1439 cm^{-1} , respectively, contribute to the experimental structure observed at approximately 1452 and 1423 cm^{-1} . The small differences between the calculated and experimental frequencies are reasonable for harmonic DFT calculations and may additionally reflect the perturbation produced by the argon matrix.

The 1400–1250 cm^{-1} region contains several modes with significant contributions from C–O stretching, O–H in-plane bending, aromatic C–H bending, and ring deformation. PA₁ and PA₃ show prominent calculated bands at 1333 and 1338 cm^{-1} , respectively. These modes are consistent with the experimental features at 1358 and 1350 cm^{-1} and indicate overlapping contributions from PA₁ and PA₃. PA₂, in contrast, exhibits a strong mode at 1292 cm^{-1} , which can be associated with the experimental band near 1310 cm^{-1} . The distinct calculated positions of these coupled C–O stretching and O–H bending modes provide additional evidence for the presence of different conformers.

Particularly strong agreement is observed in the 1200–1150 cm^{-1} region. PA₁ exhibits calculated bands at 1186 and 1176 cm^{-1} , whereas PA₃ has corresponding modes at 1188 and 1180 cm^{-1} . These modes involve predominantly C–O stretching coupled with aromatic C–H in-plane bending and ring deformation. They closely reproduce the experimental bands at 1189 and 1181 cm^{-1} . The nearly identical correspondence of both PA₁ and PA₃ with the experimental spectrum is especially significant because it indicates that the strong experimental structure in this region arises from overlapping contributions of these two conformers.

PA₂ provides a distinct contribution at lower frequency in this region. Its calculated modes at 1149 and 1141 cm^{-1} , involving predominantly C–O stretching coupled with aromatic C–H in-plane bending and ring deformation, are consistent with the experimental feature around 1136 cm^{-1} . This provides an additional spectral indication of PA₂, complementary to its characteristic carbonyl stretching band near 1713 cm^{-1} .

The region around 1120–1050 cm^{-1} provides further evidence for the coexistence of all three conformers. The PA₁ modes at 1124 and 1094 cm^{-1} , the PA₃ modes at 1108 and 1098 cm^{-1} , and the PA₂ mode at 1089 cm^{-1} contain significant contributions from aromatic C–H in-plane bending, C–O stretching, and ring deformation. Their combined contributions provide a satisfactory interpretation of the experimental band centered at 1103 cm^{-1} . Particularly noteworthy is the experimental band at 1061 cm^{-1} , which is in excellent agreement with the calculated PA₂ mode at 1061 cm^{-1} . The PA₃ mode at 1059.6 cm^{-1} provides an additional contribution at essentially the same frequency. Thus, the 1061 cm^{-1} feature represents another important region in which the calculated spectra support the simultaneous presence of more than one conformer.

Overall, the 1900–800 cm^{-1} region provides multiple independent correlations between the experimental spectrum and the calculated vibrational modes. The C=O stretching bands distinguish PA₂ from the closely related PA₁/PA₃ contributions, while the aromatic ring stretching modes, C–O stretching, O–H in-plane bending, and C–H bending modes throughout the fingerprint region provide complementary evidence. Particularly convincing correspondences are observed for PA₁/PA₃ near 1759 cm^{-1} and 1180–1190 cm^{-1} , and for PA₂ near 1713 and 1061 cm^{-1} . The combined pattern therefore strongly supports the coexistence of PA₁, PA₂, and PA₃ in the argon matrix.

Analysis of the 800–400 cm^{-1} Region

The lower-frequency region between 800 and 400 cm^{-1} was also examined in order to identify additional vibrational signatures of the three conformers (Fig. 6). In contrast to the higher-frequency fingerprint region, the calculated modes in this interval are dominated mainly by aromatic C–H out-of-plane bending, aromatic ring deformation, and coupled deformation modes involving the carboxylic acid groups. Although the experimental features are generally weaker and less resolved, several correlations with the calculated spectra are significant.

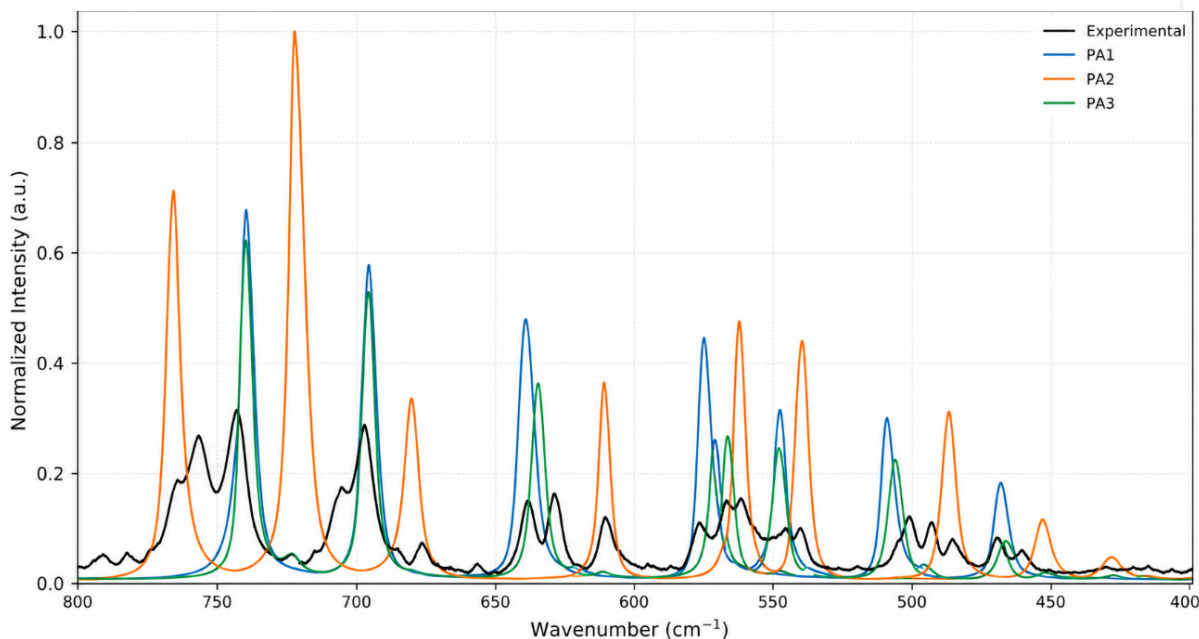


Figure 6. Experimental and calculated infrared spectra of phthalic acid (PA) isolated in an argon matrix at 15 K, covering the 800–400 cm^{-1} spectral region. The calculated spectra correspond to the PA₁, PA₂, and PA₃ conformers obtained at the B3LYP/6-311++G(d,p) level of theory. The spectral intensities were normalized for visualization and comparison of the characteristic vibrational features.

In the region around 800–730 cm^{-1} , the calculated spectra of PA₁ and PA₃ contain bands near 731–739 cm^{-1} , predominantly associated with aromatic C–H out-of-plane bending coupled with aromatic ring deformation. These modes are consistent with the experimental structure observed around 729–745 cm^{-1} . PA₂ also exhibits calculated modes at 759 and 775 cm^{-1} , which may contribute to the weak experimental structure at the higher-frequency side of this region.

A particularly significant correspondence is observed near 718 cm^{-1} . PA₂ exhibits an intense calculated band at 714.7 cm^{-1} , predominantly involving aromatic C–H out-of-plane bending and ring deformation. This mode is in excellent agreement with the experimental feature near 719 cm^{-1} , with a difference of only a few wavenumbers. Because the PA₂ band is also predicted with relatively high intensity, this correspondence provides an independent and particularly convincing spectroscopic signature for the presence of PA₂ in the argon matrix.

The experimental structure near 690–700 cm^{-1} can likewise be related to aromatic C–H out-of-plane bending and ring deformation modes. PA₁ and PA₃ both show calculated features near 695 cm^{-1} , while PA₂ has a corresponding mode at 674 cm^{-1} . The experimental profile in this region can therefore be understood as the combined contribution of conformer-specific ring deformation modes, although the relatively weak experimental intensity makes a unique assignment less certain than that of the 718 cm^{-1} band.

Another useful region occurs around 620–635 cm^{-1} . PA₁ and PA₃ exhibit calculated modes at approximately 625–629 cm^{-1} , while PA₂ has a mode at 607 cm^{-1} . These vibrations are predominantly associated with aromatic ring deformation coupled with deformation of the carboxylic acid groups. The experimental bands observed around 630–635 cm^{-1} are therefore consistent particularly well with the PA₁ and PA₃ calculations. The somewhat lower-frequency PA₂ mode may additionally contribute to the broader experimental profile.

Table 2. Assignment of the principal experimental infrared bands to the PA₁, PA₂, and PA₃ conformers of phthalic acid based on calculated vibrational frequencies.

Predominant vibrational assignment	Experimental (cm ⁻¹)	PA ₁ calculated (cm ⁻¹)	PA ₂ calculated (cm ⁻¹)	PA ₃ calculated (cm ⁻¹)
Free O–H stretching	3571.1	3571.3	3570.9	—
Intramolecular H-bonded O–H stretching	3563.1	3562.5	3562.7	3565.7
C=O stretching	1773–1767	1762.1, 1754.9	—	1754.1
C=O stretching	1759.0	1762.1, 1754.9	—	1754.1
C=O stretching	1713.0	—	1707.5, 1702.0	—
Aromatic ring C=C stretching	1607.9	—	—	1601.3
Aromatic C=C stretching / ring deformation	1590–1570	1578.1	—	—
Aromatic C–C stretching / C–H bending	1494–1484	1484.1	—	—
C–H bending / aromatic ring deformation	1452–1424	1443.1	1438.5	—
C–O stretching + O–H in-plane bending	1358–1350	1332.8	—	1338.0
C–O stretching / O–H in-plane bending	~1310	—	1292.1	1327.6
C–O stretching + aromatic C–H in-plane bending	1189.4	1186.0	—	1188.4
C–O stretching + aromatic C–H in-plane bending	1180.7	1176.4	—	1179.6
C–O stretching / C–H in-plane bending	1135.6	—	1149.5, 1140.6	—
C–H in-plane bending + C–O stretching	1102.9	1123.6, 1094.4	1089.4	1108.4, 1098.0
C–O stretching / aromatic ring deformation	1061.2	1050.0	1061.1	1059.6
Aromatic ring deformation / C–H bending	~1018	—	1017.7	—
Aromatic C–H out-of-plane bending	~800	—	774.7, 759.4	799.2, 793.6
Aromatic C–H out-of-plane bending / ring deformation	~718	737.6, 730.8	714.7	739.2, 732.8
Aromatic C–H out-of-plane bending / ring deformation	~688	—	673.7	694.8
Aromatic ring deformation + COOH group deformation	630.1	625.2, 628.8	606.8	625.2, 628.8
Ring deformation / COOH deformation	556.6	557.6, 569.6, 578.8	561.1, 552.2	554.8, 564.0
Aromatic ring deformation	~500	515.6	499.7	520.0

In the 580–550 cm⁻¹ region, several calculated modes occur for all three conformers. PA₁ has calculated bands at 579, 570, and 558 cm⁻¹, PA₂ exhibits modes near 561 and 552 cm⁻¹, and PA₃ has modes near 564 and 555 cm⁻¹. These modes mainly involve aromatic ring deformation coupled with deformation of the COOH groups. The experimental feature centered near 557–560 cm⁻¹ is therefore compatible with overlapping contributions from all three conformers. Because of the relatively broad and weak nature of this experimental feature, however, it is preferable to regard it as supporting rather than definitive evidence for individual conformers.

At still lower frequencies, calculated modes occur near 500–520 cm⁻¹ for the three conformers, with PA₂, PA₁, and PA₃ showing features around 500, 516, and 520 cm⁻¹, respectively. These modes are primarily associated with aromatic ring deformation and coupled skeletal motions. The experimental spectrum in this region is comparatively weak and less clearly resolved; consequently, these features are not used as primary evidence for conformer identification.

Taken together, the 800–400 cm⁻¹ region provides complementary support for the assignments obtained from the higher-frequency region. The excellent correspondence between the experimental feature near 719 cm⁻¹ and the calculated PA₂ mode at 714.7 cm⁻¹ is particularly noteworthy, while the bands near 695, 630, and 557–560 cm⁻¹ are consistent with calculated aromatic ring and COOH deformation modes of PA₁, PA₂, and PA₃. Although the lower-frequency region alone does not provide sufficient evidence for identifying all three conformers, its agreement with the calculated spectra strengthens the overall vibrational assignment and supports the coexistence of PA₁, PA₂, and PA₃ in the argon matrix.

5. CONCLUSION

This study presents a combined matrix-isolation FTIR and DFT investigation of the conformational landscape of phthalic acid isolated in solid argon at 15 K. Geometry optimizations at the B3LYP/6-311++G(d,p) level identified three stable conformers, PA₁, PA₂, and PA₃, corresponding to the cis/trans, cis/cis, and trans/trans orientations of the two carboxylic acid groups. The small calculated energy differences between the conformers indicate a shallow conformational potential-energy surface that allows multiple conformers to be trapped under matrix-isolation conditions.

Comparison of the calculated vibrational spectra with the experimental FTIR spectrum enabled reliable assignment of the principal infrared bands. The O–H stretching region provides the most diagnostic evidence for conformer identification: the intense experimental band at 3563.1 cm⁻¹ is primarily assigned to PA₂, the higher-frequency shoulder near 3565–3566 cm⁻¹ is consistent with PA₃, and the feature at 3571.1 cm⁻¹ is attributed to the free O–H stretching modes of PA₁ and PA₂. The characteristic C=O stretching bands of PA₂ near 1713 cm⁻¹, together with the overlapping C=O and C–O stretching bands of PA₁ and PA₃ and the

complementary assignments in the 800–400 cm^{-1} region, further support the simultaneous presence of all three conformers in the argon matrix.

Overall, the excellent agreement between the experimental and calculated spectra demonstrates that matrix-isolation FTIR spectroscopy combined with DFT calculations is a powerful approach for distinguishing closely related conformational states of phthalic acid and for providing a consistent structural and vibrational characterization of the isolated conformers.

NIR irradiation experiments were also carried out in the present study, revealing additional aspects of the conformational behavior and photochemical response of phthalic acid. Since the NIR-induced changes involve a broader and more detailed analysis than can be adequately addressed within the scope of the present work, these results are not discussed in detail here. A comprehensive evaluation of the NIR irradiation results will be presented separately in a forthcoming study and conference presentation.

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