Conference Program

First Day: Monday September 15, 2025

Time	Session	
12:00	**Arrival at the Hotel in Dahab**	
12:00-12:30	**Check-in at the Hotel**	
13:15-13:30	**S01: Opening Session**	**Group Photo**
13:30-14:30	**S02:Oral Session -01**	KNL-01-KNL-02
14:30	**Open Discussion**	
15:00	**Online Session -01** **Online Session -02**	**Science Cafe** **Poster**

Online Sessions 01&02 will beat https://www.youtube.com/@sciencecafe9129

Second Day: Tuesday September 16, 2025

Time		Session
10:00-10:30	**S03:Oral Session-02**	O-06 to O-8
10:30-12:00 **12:00 -14:15**	**S04:Oral Session-03**	KNL-03 to KNL-05 O-09 to O-17
14:15 -14:30	**Open Discussion**	
14:30-15:00 **15:00- 18:10**	**S05:Oral Session-04**	KNL-06 O-18 to O-26, O-28, O-29, O-31, O-32, O-37, O-38, O-39, O-40, O-42 and O-43
18:10-18:25	**Open Discussion**	

Third Day: Wednesday September 17, 2025

Time		Session
10:00-11:30 **11:30-13:00**	**S06:Oral Session-05**	KNL-07 to KNL-09 O-27, O-30, O-33, O-34, O- 35, O-36, O-41, and O-44
13:00-13:15	**Open Discussion**	
13:15-14:00	**Break**	
14:00-14:30	**Science Café Award Ceremony**	
14:30-15:00	**Recommendations& Closing Ceremony**	

List of Abbreviations

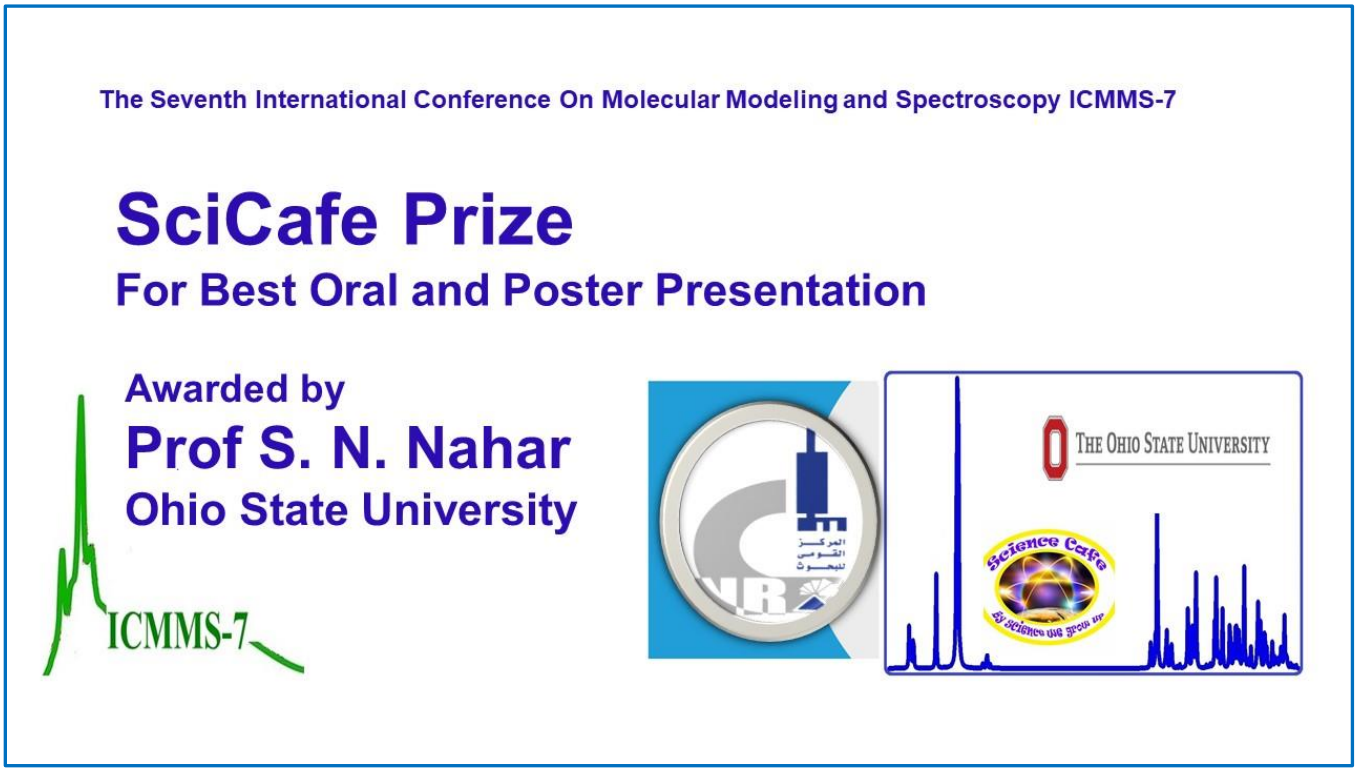
KNL: Keynote Lecture; **O**: Oral Talk; **SC**: Science Café; **P**: Poster

KNL: 30 min; **O**: 10 min

Fourth Day: Thursday September 18, 2025 - Free Tour

There will be three free tours in Dahab:

[Laguna Beach - Blue Hole – Wady Stares -Three Pools -]



Friday September 19, 2025, Departure to Cairo.

List of Keynote Lectures

No	Title
KNL-01	**To the Memory of Prof. Wolfram Baumann**
KNL-02	**Recent Trends in Raman Spectroscopy and Microscopy** Wolfram Baumann
KNL-03	**MD (Molecular Dynamics) Studies on Models of Protein-Surface Interactions** Kholmrzo T. Kholmurodov
KNL-04	**Atomic Features of Ti for Astrophysical Spectroscopy** Sultana N. Nahar
KNL-05	**Nanocomposites for Environmental Applications** Mustafa Soylak
KNL-06	**Multi-Omics Approaches in Archaeological and Archaeobotanical Remains Analyses** Nehal Sameh Ramadan
KNL-07	**Application of Molecular Spectroscopy and Molecular Modeling in the Environment and Cultural Heritage** Medhat A. Ibrahim
KNL-08	**Label-Free Vs Labelled Raman Imaging of Cells** Malgorzata Baranska
KNL-09	**Micro and Nanoplastics: New Contaminants of Soil and Water Ecosystems and Possible Solutions for Environmental Recovery** Paola Grenni

List of Orals

No	Title
O-01	**Preface: Welcome Speech Prof. Medhat A. Ibrahim** Conference Chairman
O-02	**Science Café** **Prof. Hanan Elhaes** Conference Coordinator
O-03	**Preface Welcome Speech: Welcome all of You to the Seventh International Conference on Molecular Modeling and Spectroscopy.** **Magdy Sabek** Head of Benaa Charity for Sustainable Development
O-04	**The Seventh International Conference on Molecular Modeling and Spectroscopy** **Prof. Amr Abdel Ghany** Dean of Physics Research Institute, National Research Centre, Egypt
O-05	**Preface: Welcome Speech: Welcome to You in the Sixth International Conference on Molecular Modeling and Spectroscopy** **Prof. Mamdouh Moawad** President of the National Research Centre
O-06	**Novel Composite Materials for Biomedical Applications** Yousef E. Hashem

O-07 **Evaluation of Natural Radioactivity and Environmental Impact in Agricultural Soil in the Jazan Region Using Gamma Spectra**
Entesar H. EL-Araby

O-08 **Design of a New D–π–A Discriminant Spring for Photovoltaics in Organic Solar Cells: A Study using DFT**
Amel Azazi

O-09 **Thymol: 1-octanol Deep Eutectic Solvent for Vortex-Assisted Liquid Micro extraction of Rhodamine 6G in Cosmetics**
Sabrina Sajjad

O-10 **Vortex-Assisted Micro-Solid Phase Extraction (VA-μSPE) of Pb(II) and Cd(II) from Food and Water Samples Using VMxene/ND-COOH/Bismuthene Prior to HR-CS-FAAS Determination**
Hassan Elzain

O-11 **Cobalt-Doped ZnO Modified Magnetic MWCNTs as an Efficient Adsorbent for Micro Solid Phase Extraction of Cd^{2+} and Pb^{2+} from Water and Food Matrices**
Ozgur Ozalp

O-12 **Green and Efficient Microextraction of Carmoisine Using a Carbon Quantum Dot-Based Deep Eutectic Solvent in a Hollow Fiber Membrane System**
Qamar Salamat

O-13 **New GNP@LDH nanocomposite for effective Pb(II) Extraction from the environment and food samples**
Muhammad Balal Arain

O-14 **Boron Nitride-Based $Fe_3O_4/NiWO_4$ Nanocomposites for Photocatalytic Removal of Sudan I Dye**
Nuray Güy

O-15 **Electrochemical and HPLC-Based Detection of Furosemide using Fe-Co LDH@ZIF-8 Magnetic MWCNT-Modified SPCE**
Suniya Shahzad

O-16 **Synthesizing a Novel ZnS@ZIF-8@Chitosan Nanocomposite for Trace Detection and Micro Solid Phase Extraction of Pb^{2+} in Water and Food Matrices by HR-CS-FAAS**
Abdirashid Adam Isak

O-17 **Application of $CuMn_2O_4/Dy_2O_3$ Nanocomposite in Micro Solid-Phase Extraction for Accurate Determination of Cd(II)**
Furkan Uzcan

O-18 **The Effect of Anion, Steric Factors on the Catalytic Activity of Hydrogen Peroxide, Biological Activities, Docking, and DFT Calculations of Novel Mixed Ligand of Copper Complexes**
Nelly H. Mahmoud

O-19 **On the Molecular Modeling Analysis of Hydrated Amino Acids**
Abdel Aziz Mahmoud

O-20 **Molecular Insights into the Hydration of Amino Acids**
Abdel Aziz Mahmoud

O-21 **Electronic Analyses for the Possible Hydration of Amino Acids**
Osama Osman

O-22 **Effect of Solvents on the Electronic Properties of Polyvinyl Chloride**
Hanan Elhaes

O-23 **Modeling Graphene Oxide Decorated with FeO, SO, and NO**
Hesham El Meligy

O-24 **Investigating the Electronic Properties of Graphene Oxide Functionalized with Benzoic Acid**
Medhat A. Ibrahim

O-25 **Role of Humic Acid in the Coordination of Cd, Cu, and Pb: A DFT Approach**
Medhat A. Ibrahim

O-26 **Modeling Intermolecular Complexes of Small Organic Molecules with CO_2 and H_2O Using DFT**
Hanan Elhaes

O-27 **Application of Graphene Oxide/Polypyrrole/Zinc Oxide Nanocomposites for Amino Acid Sensing**
Nada A. Khaled

O-28 **Application of Cs/GO/TiO_2 as a Gas Sensor**
Amged G. El-Srougy

O-29 **Functionalized Reduced Graphene Oxide via Metal Decoration as Humidity Sensor**
Khaled S. Amin

O-30 **Spectroscopic Analyses for Possible Transport of Pollutants into Fish**
Medhat A. Ibrahim

O-31 **DFT-Based Evaluation of Modified Graphene Quantum Dots for HIV-1 Protease Inhibition**
Abdel Aziz Mahmoud

O-32 **Astrophysical Spectral Analysis Expansion of the Universe and Spectroscopic Identification of Z-Shifted Lines Observed by JWST**
Shreyas Thummala

O-33 **Lithium Battery Recycling: Overview and a New Direction**
Tae-Sik Oh

O-34 **Modeling the Functionalized Genistein-Hyoscyamine Derivatives**
Rana Abd-ElSalam

O-35 **Interaction Analysis of Guanine-based Structure**
Islam Gamal

O-36 **Molecular Modeling Analysis for Functionalized Sodium Alginate/ Polypyrrole/Titanium Dioxide**
Amira M. Salem

O-37 **Elucidating the Electronic Properties of Chitosan/Hydroxyapatite/Graphene Oxide**
Dina Shehata

O-38 **Development and Characterization of a Graphene-Based Nanocomposite Gas Sensor for Room-Temperature CO and CH_4 Detection**
Manar Sobhy

O-39 **Investigating the Electronic Properties of PANI/Graphene/PVDF/PTFE Nanocomposite**
Aya Allah Mahmoud

O-40 **Enhancing the Structural and Optoelectronic Properties of Carboxymethyl Cellulose Sodium Filled with ZnO/GO and CuO/GO Nanocomposites for Antimicrobial Packaging Applications**
Rania Badry

O-41	**DFT Study of Beetroot Carbon Dots-Cellulose Sulfate Film for Chromium and Bacterial Detection in Tomatoes** Hebat-Allah S. Tohamy
O-42	**Enhanced Energy Storage Performance of Al-Doped $BaZr_{0.2}Ti_{0.8}O_3$ Ferroelectrics Prepared by Sol-Gel Processing** Ali B. Abou Hammad
O-43	**Sol-Gel Derived Lead-Free $BaZr_xTi_{1-x}O_3$ Ferroelectric Ceramics for High-Performance Energy Storage Applications** Amany M. El Nahrawy
O-44	**Application of Chitosan/Graphene and Chitosan/Graphene Oxide Composites for Removal of Cu and Pb** Abdel Salam El-Sheikh

List of Posters

No	Title
P-01	**Fate and Impact of Heavy Metals in the Environment** Mohamed S. AbdelAal
P-02	**Recent Developments and Progress in Functionalized Biomaterials** Osama Osman
P-03	**Application of Chitosan as a Bio-Carrier for Protein** Yasmine O. Osman
P-04	**Introduction to the Environmental Applications of Chlorella** Basmaa K. Farghly
P-05	**Effect of Graphene on the Structural and Optical Properties of CMC** Rania Badry
P-06	**Biomaterials as Composite Materials for Teeth Filling Applications** Yousef E. Hashem
P-07	**Functionalized Recycled Polyethylene Terephthalate for Several Applications** Amr Antar
P-08	**Optimization of Cost-Effective Handmade Electrospun** Medhat A. Ibrahim
P-09	**How and Why Measure Excited State Dipole Moments of Solute Molecules?** Wolfram Baumann
P-10	**Optimization of PET/rGO Nanocomposite for Removal of Zn from Wastewater** Mohamed S. AbdelAal
P-11	**Simple Route for Possible Remediation of Zinc with Chitosan** Asmaa Ibrahim
P-12	**Artificial Intelligence (AI) Assisted PET/rGO as Flexible Substrate** Sheimaa Ibrahim
P-13	**Artificial Intelligence (AI) AssistedrGO for Water Splitting** Haitham Shabaan
P-14	**Artificial Intelligence (AI) Assisted for Novel CO_2 Capture** Fatma Mohamed

P-15	**Exploring Materials from the Local Egyptian Environment by Consulting Artificial Intelligence (AI)** Essam Ehab
P-16	**Artificial Intelligence (AI) as a Tool for Environmental Protection Assessment** Seif Eldin Mohamed
P-17	**Protection of the Environment with Traditional Methods in Rural Areas** Benaa Charity
P-18	**Water Management in Urban Areas Assisted by Artificial Intelligence (AI)** Benaa Charity
P-19	**Waste Management in Urban Area Assisted by Artificial Intelligence (AI)** Benaa Charity
P-20	**Preservation of Cultural Heritage Assisted by Artificial Intelligence (AI)** Benaa Charity
P-21	**Modeling and Experimental Analyses for Chitosan/Zinc Oxide Nanocomposite** Hanan Elhaes
P-22	**AI-Driven DFT Modeling of Graphene Oxide–TiO_2 Nanocomposites** Amged G. El-Srougy
P-23	**AI-Assisted Material Selection and DFT Analysis of HA/GO/MnO_2 Composites for Supercapacitor Electrodes** Mahmoud S. Ghanem
P-24	**Spectroscopic Analyses of Lead in Water using Dispersive Liquid–Liquid Microextraction** Mohamed Abdel Aaal
P-25	**Modeling the Effect of Solvents on the Electronic Properties of C_{60}** Asmaa Ibrahim
P-26	**Non-Destructive Spectroscopic Analysis of Coptic Icons** Osama Osman

Science Café

No	Title
SC-01	**Science for the Society: Science Café**
SC-02	**Molecular Modeling and Molecular Spectroscopy Group at National Research Center**
SC-03	**Molecular Modeling Group at Faculty of Women for Arts , Science and Education, Ain Shams University**
SC-04	**Science and Technology in the Time of Artificial Intelligence**
SC-05	**An Introduction to Artificial Intelligence (AI)**
SC-06	**Machine Learning and Artificial Intelligence AI**
SC-07	**Molecular Modeling Features and Applications**
SC-08	**Application of AI in Molecular Modeling**
SC-09	**Artificial Intelligence AI, Machine Learning ML and Molecular Modeling MM**
SC-10	AI-Assisted **of DFT Applications in Protein Interaction**
SC-11	**AI-Assisted DFT Modeling of Polysaccharides**
SC-12	**AI-Assisted Applications for DFT Modeling of Polysaccharides**
SC-13	**AI-Assisted Applications of DFT Modeling of Nanometal Oxides**
SC-14	**AI-Assisted Modeling of Carbon-Based Materials**

SC-15	**AI-Assisted Applications for DFT Modeling of Carbon-Based Materials**
SC-16	**Application of AI and ML in Environment and Cultural Heritage**
SC-17	Application of AI in the Assessment of Heavy Metals
SC-18	**Application of AI in the Removal of Heavy Metals**
SC-19	Application of AI in the Assessment of Organic Pollution
SC-20	**Application of AI in the Removal of Organic Pollution**
SC-21	Application of AI in Studying the Effect of Climate Changes upon Soil
SC-22	**Application of AI in Controlling the Effect of Climate Changes**
SC-23	**Application of AI in Studying the Effect of Climate Changes upon River Water**
SC-24	**Application of AI in Studying the Effect of Climate Changes upon Sea Water**
SC-25	**Application of AI in Cultural Heritage**
SC-26	**Application of AI in the Restoration of Metal Artifacts**
SC-27	**Application of AI in the Restoration of Wooden Artifacts**
SC-28	**Application of AI in the Restoration of Wall Painting**
SC-29	**Introduction to Photogrammetry and Image Processing**
SC-30	**Photogrammetry and Artificial Intelligence AI**