List of Keynote Lectures

No	Title
KNL-01	**Computational Molecular Spectroscopy** **Prof. Medhat A. Ibrahim**
KNL-02	**Advancing Healthcare with 3D Printing: From Custom Implants to Bioprinting** **Dr. Nayera M. El-Sayed**
KNL-03	**Innovation and Opportunities in Developing Molecules for the Agrochemical and Defense Industries: From Theory to Technology** **Prof. Teodorico C. Ramalho**
KNL-04	**Microbial Biodiversity and Energy Production in Terrestrial Microbial Fuel Cells: Effects of Compost as an Organic Amendment** **Prof. Paola Grenni**
KNL-05	**X-crystallography and its applications in biomaterials** **Prof. Ahmed F. Mabied**
KNL-06	**Spectral Features of Ions of Lanthanides for Kilonovae** **Prof. Sultana N. Nahar**
KNL-07	**Negative Ion Resonances Lifetime and Electron Loss Cross Sections at Low Energy Interactions.** **Prof. Guillermo Hinojosa**
KNL-08	**The Solar Problem: Element Abundances and Opacities** **Prof. Anil Pradhan**
KNL-09	**Spray Dried Hollow Carbon Spheres from Lignin: Adsorption Kinetics and Thermodynamics Study for Highly Efficient Wastewater Treatment** **Prof. Tae Sik Oh**

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 in the Sixth Hybrid International Conference on Molecular Modeling and Spectroscopy.** **Magdy Sabek** Head of Benaa Charity for Sustainable Development
O-04	**The Sixth Hybrid 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 all of you in the Sixth International Conference on Molecular Modeling and Spectroscopy**

Prof. Mamdouh Moawad
President of the National Research Centre

O-06 **Design of Gas Sensor Based on Graphene Oxide/ZnO/Polyvinylidene Fluoride**
Manar Sobhy

O-07 **Laser Irradiation for Graphene Oxide/ZnO/ Polyvinylidene Fluoride as a Gas Sensor Application at Room Temperature**
Manar Sobhy

O-08 **Novel metal complexes of N^1, N^2-bis(4-phenylthiazol-2-yl)phthalamide: Synthesis, spectroscopic, thermal and kinetic investigations, molecular modeling, computational calculations, anti-breast cancer studies**
Nelly H. Mahmoud

O-09 **Estimation of Radioactive Nuclei in Building in Jazan**
Entesar H. EL-Araby

O-10 **Modeling and Quantum Chemical Studies of Halogenated Pyrazole-Benzamides: DFT Insights into Anticancer Activity and EGFR Inhibition**
Nada A. Khaled

O-11 **The Effect of the Additive of rGO on the Dielectric and Impedance Spectroscopy Studies of the $Ba_{0.9}Sr_{0.1}Ti_{0.9}Zr_{0.1}O_3$ Ceramics**
Ahmed I. Ali

O-12 **Spectral Characterization and Elemental Composition of Early Universe Galaxy using JWST Near-Infrared Spectroscopy(NIRSpec)**
Vidit Bhandari

O-13 **Heating Mechanisms of the Solar Corona: The Past, Present, and Future.**
Azalea Shillington

O-14 **Process Safety and Environmental Protection**
Ahmed Abdel-Karim

O-15 **A Novel Three-Phase Hollow Fiber Liquid Phase Microextraction Method Employing Deep Eutectic Solvents for the Simultaneous Extraction of Cationic, Anionic, and Nonionic Dyes from Water and Food Samples**
Sabrina Sajjad

O-16 **Investigating the Electronic Properties and Reactivity of Polyaniline Emeraldine Base Functionalized with Metal Oxides**
Medhat A. Ibrahim

O-17 **Application of Polyvinyl Alcohol/ Sodium Alginate Electrospun Nanofibers as Biosensor**
Ahmed Fahmy

O-18 **Effect of Glycerin on the Physical Properties of Polyvinyl Alcohol/ Sodium Alginate Blend**
Ahmed Fahmy

O-19 **Investigating the Electronic Properties of Edge Glycine/Biopolymer/Graphene Quantum Dots**
Nayera M. El-Sayed

O-20 **Molecular Modeling Analysis for Functionalized Graphene/Sodium Alginate Composite**
Medhat A. Ibrahim

O-21 **Design, Characterization and Implementation of Cost-effective Microspheres for Remediation of Divalent Metals from Wastewater**

Medhat A. Ibrahim

O-22 **Human Metabolites as a Source for ABCB1 Inhibitors: A Comprehensive Study Using Machine Learning-Enhanced Virtual Screening and Molecular Dynamics Simulations**
Khlood A. A. Abdeljawaad

O-23 **Modeling the Effect of Metal Oxides on the Electronic Properties of PVDF**
Hanan Elhaes

O-24 **Application of Functionalized Graphene Quantum Dots with ZnO as a Humidity Sensor**
Asmaa Ibrahim

O-25 **Modeling the Electronic Properties of Acetylsalicylic Acid**
Yasmine O. Osman.

O-26 **Microdrop InkJet Printed Supercapacitors of Graphene/Graphene Oxide Ink for Flexible Electronics**
Ahmed M. Bayoumy

O-27 **Biomaterials and Physics of Bio Glass Applications**
Taha Tiama

O-28 **Insights into Structural, Dielectric, Optical and Ferromagnetic Properties of Cesium Ferrate (Cs_2FeO_4) Nanorods via Bottom-Up Synthesis**
Fawzy G. El Desouky

O-29 **Temperature-Dependent Study of Electrical, Optical, and Luminescent Properties in Perspective Oxostannate $Cs_2Sn_2O_3$ Nanostructures**
Fawzy G. El Desouky

O-30 **Synthesized One-Step Recyclable and Biodegradable Ag@Chitosan Nanocomposite Beads for Catalytic Hydrogenation of 4-Nitrophenol**
Asmaa M. Ismail

O-31 **Optical Bandpass Filter Customization in Sodium Silicate Glass: Effect of Incorporating CuO**
Gehad O. Rabie

O-32 **UV–Vis Studies of ItO glass Coated with Cellulose Acetate Film Blended Different Concentrations of MoO_3-NPs**
Dina Ezzat

O-33 **Graphene-Enhanced S390 High-Speed Steel: A New Horizon in Advanced Material Design Using Powder Metallurgy**
Hadier M. Zidan

O-34 **Application of Biomaterials in Environment and Drug Delivery Systems**
Ahmed Refaat

O-35 **Modeling of SFS phi-0 Josephson Junction.**
Yury M. Shukrinov

O-36 **Stable States of Magnetization and Switching between them in the SFS Junction on the Surface of a 3D Topological insulator**
Ilhom R. Rahmonov

O-37 **Application of PLA/GO/ZnO and PLA/GO/Cu_2O as Sensor**
Yahia M. Abdallah

O-38 **Design and Implementation of PLA/GO/ZnO and PLA/GO/CuO as CO_2 Sensor**
Khaled S. Amin

O-39 **Studying the Electronic Properties of SiO_2/GO/Pb_3O4/Bi_2O_3**

	Nabil S. Abdelaziz
O-40	**Modeling the electronic properties of chitosan/hydroxyapatite/graphene oxide** **Dina Shehata**
O-41	**Heavy Metals Contamination in the Environment** **Abdel Aziz Mahmoud**
O-42	**Biomedical Applications of Functionalized Biomaterials** **Osama Osman**
O-43	**Modeling the complexation of hydrated lead and -1,3,4Thiadiazole-2,5-dithiol** **Abdel Aziz Mahmoud**

List of Posters

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P-02	**Enhancing the Structural, Optical, Electronic, and Antibacterial Activity of Carboxymethyl Cellulose Sodium Filled with ZnO/GO and CuO/GO Nanocomposites and Their Potential Application in Antimicrobial Packaging** **Noha M. Sabry**
P-03	**Role of SiO_2, TiO_2, and Fe_3O_4 Adsorbed on Glycine for Remediation of Heavy Metals and Antibacterial Activity in Water** **Rania Badry**
P-04	**Fullerene Derivatives as HCV NS5B Inhibitors** **Eman H. EL-Sakhawy**
P-05	**Modeling the Effect of Metal Substitutions Upon Fullerene** **Abdel Aziz Mahmoud**
P-06	**Cu_2O-Doped Phosphate Glasses as Bandpass Filter** **Asmaa Ibrahim**
P-07	**On the Spectroscopic Analyses of Water Hyacinth** **Fatma Atia**
P-08	**Mapping Electrostatic Potential of Fullerene: DFT Approach** **Medhat A. Ibrahim**
P-09	**Design and Implementation of Cutting Machine for Plastic Control** **Amr Antar**
P-10	**Global Reactivity Descriptors and Thermal Analyses of Polyethylene Terephthalate Interacted with Cd and Pb** **Amr Antar**
P-11	**Application of PLA/GO/NiO as Ammonia Sensor** **Khaled S. Amin**
P-12	**Modeling the Interaction between Chitosan/Graphene and Di-Hydrated Lead** **Abdel Salam El-Sheikh**
P-13	**Waste Control and Management** **Benaa Charity**

P-14	**Plastic Control and Management** **Benaa Charity**
P-15	**Plastic Control and Management Strategies and Aspects** **Benaa Charity**
P-16	**Saving Water at Home** **Benaa Charity**
P-17	**Controlling the Ibuprofen in Aqueous Solution using Natural Microspheres** **Ahmed M. Bayoumy**
P-18	**Modeling and Spectroscopic Analyses for the Effect of Salinity on Soil** **Asmaa Ibrahim**

Science Café

No	Title
SC-01	**Science for the Society: Science Café**
SC-02	**Molecular Modeling and Molecular Spectroscopy Group at National Research Centre**
SC-03	**Molecular Modelling Group at Faculty of Women for Arts, Science and Education, Ain Shams University**
SC-04	**Carbon Based Materials**
SC-05	**Carbon Based Materials: Graphite**
SC-06	**Carbon Based Materials: Diamond**
SC-07	**Carbon Based Materials: Fullerenes**
SC-08	**Carbon Based Materials: Carbon Nanotubes (CNTs)**
SC-09	**Carbon Based Materials: Graphene**
SC-10	**Carbon Based Materials: Amorphous Carbon**
SC-11	**Carbon Based Materials: Carbon Fibers**
SC-12	**Carbon Based Materials: Glassy Carbon**
SC-13	**Carbon Based Materials: Carbon Foam**
SC-14	**Carbon Based Materials: Carbon Quantum Dots**
SC-15	**Applications of Carbon Based Materials**
SC-16	**Applications of Carbon-Based Materials in Electronics**
SC-17	**Applications of Carbon-Based Materials in Optoelectronic Devices**
SC-18	**Applications of Carbon-Based Materials in Energy Storage and Conversion**
SC-19	**Applications of Carbon-Based Materials in Composites and Materials Science**
SC-20	**Applications of Carbon-Based Materials in Biomedical Applications**
SC-21	**Applications of Carbon-Based Materials in Environmental Applications**
SC-22	**Applications of Carbon-Based Materials in Catalysis**
SC-23	**Applications of Carbon-Based Materials in Sensors**
SC-24	**Applications of Carbon-Based Materials in Agriculture**