

Conference Program

First Day: Sunday - December 18, 2022

Time	Session	
09:00	Registration	
10:00	S1: Opening Session	O-01 to O-05
10:30	S2: Oral Session-1	KNL- 01 O-06 to O-13
12:10	Open Discussion	
12:30	Break	
13:15	S3: Oral Session-2	KNL-02 O-14 to O-18
14:40	Open Discussion	
15:00	S4: Oral Session -3	KNL-03 O-19 to O-25
16:40	Open Discussion	
17:00	Side Event-1 Science Café Channel	Sustainable Development

Second Day: Monday - December 19, 2022

Time	Session	
09:00	S05: Oral Session -4	KNL-04 to KNL-05 O-26 to O-29
11:00	Open Discussion	
11:20	S06: Oral Session -5	KNL-06 O-30 to O-34
12:40	Open Discussion	
13:00	Break	
13:45	S07: Oral Session-6	KNL-07 O-35 to O-39
15:05	Open Discussion	
17:00	Side Event-2 Science Café	Science Café Channel

Third Day: Tuesday - December 20, 2022

Time	Session
09:00	S08: Oral Session -7 KNL-08 to KNL-10 O-40
10:45	Open Discussion
11:00	S09: Side Event-3 Wein2K Workshop KNL-11 on Science Café O-41 to O-46
12:10	Break
13:00	Poster Session* Open Discussion P-01 to P-50
16:00	Recommendations & Closing Ceremony

***Poster Session will be all the day on Science Café channel**

List of Abbreviations

KNL: Keynote Lecture

O: Oral Talk

SC: Science Cafe

SD: Sustainable Development

P: Poster

List of Keynote Lectures

No	Title
KNL-01	Recent Application of the Molecular Spectroscopy and Modeling Unit at NRC., Egypt Prof. Medhat A. Ibrahim
KNL-02	Hydrogels: The Soft Magic of Bioprinting Prof. Wafaa I. Abdel-Fattah
KNL-03	Recent Applications of Laser Spectroscopy and LIDAR to Minimize Climate Changes and Environmental Pollution Prof. Walid Tawfik
KNL-04	Laser Induced Fluorescence Prof. Lotfia M. EL Nadi
KNL-05	Metal Organic Frameworks and their Nanocomposites in Solid Phase Extraction Studies Prof. Mustafa Soylak



KNL-06	Opportunity of High Value-Added Advanced Materials from Secondary Resources and Low-Grade Raw Materials Prof. Mohamed M. Rashad
KNL-07	Nature Based Solutions for Recovering Contaminated Sites Prof. Paola Grenni
KNL-08	Chlorine Spectra for Astrophysical Modeling Prof. Sultana N. Nahar
KNL-09	Critical Evaluation and Compilation of Atomic Data Prof. Haris Kunari
KNL-10	A New Spectrometric Species: The History of its Finding and its Confirmation Prof. Guillermo Hinojosa
KNL-11	The significance of Computational Tools in Materials Science: Brief Overview Prof. Saad Tariq

List of Oral Talks

No	Title
O-01	Preface: Welcome Speech Prof. Medhat A. A. Ibrahim Conference Chairman
O-02	In the Memory of Prof. Ahmed Fakhry
O-03	Preface Welcome Speech Magdy Sabek Head of Benaia Charity for Sustainable Development
O-04	The Fourth Hybrid International Conference on Molecular Modeling and Spectroscopy Prof. Aisha Moustafa Acting Dean of Physics Research Institute
O-05	Preface Welcome Speech Prof. Hussein Darwish President of National Research Centre
O-06	Development of Carboxymethyl Cellulose Sodium/CuO Nanocomposite Films with Structural and UV-Blocking Properties Rania Badry
O-07	Investigating Thermal Behavior of Polymer Networks Based Acrylic Monomers through Atomistic Molecular Dynamics Simulations Ahlam Benkhelifa
O-08	Recent Advances in Sensors Ahmed Refaat
O-09	Studying the Optical and Thermal Properties of Cs/ZnO and Cs/ZnO/GO Hybrid Nanocomposites Hend A. Ezzat

- O-10 Developing Two Ionic Derivatives of Chitosan: Structure and Dynamic Properties Relationships
Fathia M. E. Mohamed
- O-11 The Influence of Additions of Molybdenum Trioxide Nanoparticle on the Structural and Optical Properties of Cellulose Acetate Film
Dina Ezzat Mahmoud
- O-12 DFT Study about the Sensitivity of Reduced Graphene Oxide to Cholesterol Lipid Structure
Abdel Aziz Mahmoud
- O-13 Effect of CuO on the Structural, Optical and Electronic properties of PVP: Experimental and DFT Study
Naglaa Shahin
- O-14 Nanometal Oxide/Biopolymer Composite Scaffolds for Nerve Cells Regeneration
Hanan Beherei
- O-15 Intermediate Water as a New Tool for the Prediction of Materials Biocompatibility
Mostafa Mabrouk
- O-16 Novel Cost Effective Skin Regenerative Hydrogel Patch for Wound Healing
Mona Moaness
- O-17 Magnesium Phosphate Nano-Fillers for Bone Regeneration
Sara Ali Mohamed El-Sayed
- O-18 Variations in Morphological Traits, Net Photosynthesis and Expression of Some Genes, and their Relation to Drought Resistance of Seven Rice Genotypes.
Gehad M. A. A-R. El-Ezaby
- O-19 Accurate Consideration of Stark Broadening Parameters of Aluminum using Ultrafast Laser Spectroscopy
Mohamed Fikry
- O-20 Assessment of Different Technologies for the Adsorption of Atrazine in Polluted Water
Ahmed Hellal
- O-21 Spectroscopic Consideration of Pollution Index, Bioaccumulation Factor, Health Risk Index, and Daily Intake of Heavy Metals in Environmental Samples from North Delta Egypt
Noura Fayek
- O-22 Plasma Characterization of Calcium in Lettuce and Clover Plants from Different Locations in Egypt Using Picosecond Laser-Induced Breakdown Spectroscopy
Noura Fayek
- O-23 Determination of Saturated and Unsaturated Hydrocarbons in Petroleum Oil Pesticides using FTIR Spectroscopy
Mohamed Abdelgwad
- O-24 Carbamazepine Removal from Contaminated Water via Different Adsorption Methods
Nada Ahmed
- O-25 Supramolecular Light Harvesting Donor-Acceptor Complexes: Laser Photolysis Studies
Mohamed E. El-Khouly

- O-26 Synthesis of ZnO/CNT@ Fe₃O₄ Nanocomposite FOR Magnetic Solid Phase Microextraction of Rhodamine B in COSMETICS and Plastic Products
Nebiye Kizil
- O-27 An Innovative Zn@MoO₃ nanorods for Solid Phase Extraction and Determination of Lead in Food and Water Samples Combined with High-Resolution Continuum Source Atomic Absorption Spectrometry (HR-CS-AAS)
Furkan Uzcan
- O-28 A MWCNTs@CuAl₂O₄@SiO₂ Nanocomposite for the Speciation of Chromium in Natural Water Samples Prior to High-Resolution Continuum Source Flame Atomic Absorption Spectrometric (HR-CS-FAAS) Determination
Hassan Elzain H. Ahmed
- O-29 Switchable Hydrophilicity Solvent Based Liquid-Liquid Extraction of Pd(II) from Environmental Samples
Ozgun Ozalp
- O-30 Investigation of the Effect of Aluminum on the Structural, Compositional, Morphology, Optical and Photocatalytic Properties of ZnO-GO Nanocomposites
Talaat A. Hamid
- O-31 Smart Electronic Power Saving Systems
Merna A. Tawfik
- O-32 Applicable Physical Characteristics of Pulsed Laser Deposited In_{1-x} Pb_x Se Thin Film Alloys
Hesham A. Elmeleegi
- O-33 Synergistic effect of tin ferrite on ZnSnO_{3-x} nanostructures: Xay photoelectron spectroscopy and photoluminescence study
Fawzy G. El Desouky
- O-34 Green Chemistry Driven Synthesis of Bismuth-based Perovskites as an Efficient Absorber Material for Solar Cell Applications
Moamen R. A. Elsayed
- O-35 Interaction of Biopolymers with Graphene for Bioelectronic Applications
Ahmed M. Bayoumy
- O-36 Effect of Metal Oxide Additives on the Structural, Morphology and Dielectric Properties of BaTiO₃ for Capacitors Application
Sahar Sallam
- O-37 Bioremediation of Congo Red Dyes Using Biosynthesized Copper/Iron Nanoparticles
Mai Taha
- O-38 Isolation and Characterization of Endophytic Bacteria from Parts of the Aquatic Halophyte *Cyperus laevigatus* L. Collected from Wetland
Yasser A El-Amier
- O-39 Chemical Composition of *Halocnemum strobilaceum* Methanolic Extract and Its Potenti Antioxidant and Cytotoxic
Shahenda M. El-Afify
- O-40 PII Biosignature Line Ratios in Exoplanetary and Nebular Environments
Kevin Hoy
- O-41 DFT calculations of NdMO₃ (M=Fe, Co, and Mn) Perovskite Structure Using Wien2k Code

Shaban I. Hussien

O-42 Elucidating the effect of magnetic attributes of $\text{Nd}_{0.5}\text{Sr}_{0.5}\text{MnO}_3$: A DFT Overview

Ihab A. Abdel-Latif

O- 43 Studying the Effect of Pressure on Physical Attributes of Ferromagnetic PrMnO_3 for Spintronic Device Applications: DFT-GGA Calculations

Saad Tariq

O- 44 Elucidating the Influence of Exchange-correlation Functional on Ferromagnetic Attributes of PrVO_3 for Magneto-optical Sensors

Ihab A. Abdel-Latif

O- 45 The Photocatalytic Performance of the Perovskites: DFT Study

Ihab A. Abdel-Latif

O-46 Theoretical Investigations on Physical Properties of $\text{Nd}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$

Shaban I. Hussien

Side Event-1: Science Café

No	Title
SC-01	Science for the Society: Science Cafe
SC-02	Molecular Modeling and Molecular Spectroscopy Group at National Research Centre
SC-03	Molecular Modeling Group at Faculty of Women for Arts, Science and Education, Ain Shams University
SC-04	Nano NRIAG Unit at the National Research Institute of Astronomy and Geophysics.
SC-05	Introduction to Molecular Modeling
SC-06	Introduction to Density Functional Theory DFT
SC-07	Building Model Molecule
SC-08	Running the Calculations
SC-09	Molecular Modeling Could Assign Normal Mode of Vibration
SC-10	Vibrational Assignment for Acetic Acid
SC-11	Spectroscopy
SC-12	Molecular Spectroscopy
SC-13	Fourier Transform Infrared Spectroscopy FTIR
SC-14	Some Applications of FTIR
SC-15	FTIR Spectral Interpretation
SC-16	Raman Spectroscopy
SC-17	Difference between Raman Spectroscopy and IR Spectroscopy
SC-18	Advantages of Raman Spectroscopy
SC-19	Molecular Imaging
SC-20	FTIR Imaging
SC-21	Raman Imaging

Side Event-2: Sustainable Development

No	Title
SU-01	General Introduction for Sustainable Development
SU-02	Interconnected and Ambitious Goals of Sustainable Development
SU-03	Egypt: Sustainable Development Knowledge Platform Voluntary National Review 2021
SU-04	Sustainable Development Strategy in Egypt... Prospects and Challenge
SU-05	Civil Society's Major Role in Sustainable Development
SU-06	Expanding Opportunities for the Egyptian Private Sector in the Post-COVID Era
SU-07	COP27 presents Egypt Financing Opportunities for Sustainable Development
SU-08	Role of Bena Charity Organization in Sustainable Development in Qalyobia Governorate

Side Event-3: WIEN2k Soft Code Workshop

KNL-11; O-46 to O-51

List of Posters

No	Title
P-01	Computational Notes on the GQDs: AH ₆ C ₄₂ Substituted by P, As, and Sb atoms Osama Osman
P-02	Modeling of Structural, Electronic and Mechanical Properties of 3D Rutile Type SnO ₂ by Hybrid Density Functional Theory Ibrahim Moussa
P-03	Electronic Properties of Graphene Quantum Dots Substituted with Al, Ga and In Medhat A. Ibrahim
P-04	DFT Calculations for Graphene Quantum Dots Filling with Al, Ga, In Abdel Aziz Mahmoud
P-05	Effect of Hydration on the Physical Properties of Graphene Quantum Dots Medhat A. Ibrahim
P-06	Computational Notes on the GQDs: ATRI, AH ₆ C, ZTRI, and ZHEX Substituted Nitrogen Hanan Elhaes
P-07	On the Substitution of Al, Ga and In with the Graphene Quantum Dots Hanan Elhaes
P-08	Modeling Study of (Al, Ga and In)- Substituted Graphene Quantum Dots Osama Osman
P-09	Ability of Trihalomethanes Sensing using Functionalized 2D MXene Ti _{n+1} C _n T _n (T=F, Cl, O and OH)

- Islam Gomaa**
- P-10 Computational Notes on the ZHEX C₅₄ Substituted by P, As, and Sb atoms
Asmaa Ibrahim
- P-11 Porous stainless-steel nanocomposite for medical applications: Preparation, Characterization, Dielectric Properties, Biological Evaluation, and Liability Detection of Immunogenicity
Ahmed I. Ali
- P-12 On the Molecular Spectroscopic Analyses of Chitosan/Fe₃O₄ Nanocomposite
Asmaa M. Ismail
- P-13 Utilization of Graphyne (Gy) instead of Graphene(G) for electrons direction control: Theoretical approaches of electronic Comparison between Gy and G
Islam Gomaa
- P-14 Convalescent plasma therapy
Ghada Tourky
- P-15 Infrared Spectral Studies Analysis of Barium-Nickel Ferrite Doped by Zinc
Sadiq Hassan Yahya Khoreem
- P-16 Phytochemical Analysis, Antioxidant and Antimicrobial Activities of Emergent Cyperus laevigatus L
Yasser A El-Amier
- P-17 Assessing the optical characteristics of nano-composite CMC/PVP thin films embedded in green synthesized silver nanoparticles
Magdy Elsaady Abo elwafaa Dawood
- P-18 Assessment the Physico-Chemical Characteristics of Sediment in Bardawil Lagoons, Egypt
Wafaa K. Kotb
- P-19 Energy storage: overview and outlooks
Esraa Soliman
- P-20 Computational Notes on the Effect of Li, Na and K on the Vibrational Spectra of Fatty Acid
Shimaa Gamal
- P-21 Development of Mechanical and Physical Properties of Material Using New Radiated Ferrous Alloy
Yasser H. El-Shaer
- P-22 Glucose Sensing Utilizing Biosensor Based on Graphene Oxide/ ZnO/ Polyvinylidene Flouride: A DFT Approach
Manar Sobhy
- P-23 Electronic Modification of PVDF Hybrid Membranes: Experimental and Theoretical Approaches
Amina Omar
- P-24 PMMA/PVDF Hybrid Membranes Reinforced with 2D ZnO and GO: Theoretical and Experimental Approaches
Amina Omar
- P-25 Needle-Sphere 2D rGO/alginate Matrix for Unusual prolonged release of Cefotaxime
Islam gomaa

- P-26 Electronic Properties and Molecular Electrostatic Potential Mapping of GQDs Decorated with ZnO, CuO, and TiO₂
Asmaa Ibrahim
- P-27 Computational notes of Catechol-O-methyltransferase (COMT) Inhibitors for Parkinson's Disease Treatment
Salma S. Younes
- P-28 Molecular Modeling Approach of Effect of Graphene Oxide, Titanium Oxide and Silicon Oxide on Phospholipids Membranes
Amina Omar
- P-29 Functionalized Alumina Nanoporous Membrane for Neural Diseases Treatment
Nouran Esmat
- P-30 Role of silver nanoparticles on the structure and optical properties of CS/PVP/AMOX nanocomposite
Samar Ebrahim
- P-31 PARP-1 inhibition, apoptosis induction, and cell cycle analysis of leukemia cells treated with novel 1,2,3-triazole chalcone hybrids
Ebtehal M. Hussein
- P-32 Structure based design and synthesis of 3-(7-nitro-3-oxo-3,4-dihydroquinoxalin-2-yl) propanehydrazide derivatives as novel bacterial DNA-gyrase inhibitors: In-vitro, In-vivo, In-silico and SAR studies
Rogy R. Ezz Eldin
- P-33 Synthesis, cytotoxicity evaluation of some novel benzochromene, benzochromenopyridine, and benzochromenopyrimidine derivatives
Fatma G. Abdul Rahman
- P-34 Cardiovascular Protection: Atherosclerosis
Saied Elwy
- P-35 Synthesis, DFT calculations, *In silico* studies, and biological evaluation of pyrano[2,3-*c*]pyrazole and pyrazolo[4',3':5,6]pyrano[2,3-*d*]pyrimidine derivatives
Mohamed G. Abouelenein
- P-36 Soft Modification of sawdust as an effective Agro-waste for promising degradation of brilliant blue and Amoxicillin
Safaa R. Fouda
- P-37 Vanadium-doped MnO₂ nanocatalyst for visible-light-driven photodegradation of selected fluoroquinolone antibiotics from contaminated water
Rafi O Zaman Brohi
- P-38 Competitive and Sustainable Removal of Iron (II) from Water by Seaweed Antioxidants Sargassum Filipendula, Spectrophotometric Detection
Menna M. El-Beshlawy
- P-39 Application of Carboxymethyl Cellulose Sodium/CuO Nanocomposites as a Sensor for NH₃ and H₂S Gases: Modeling Approach
Nadra Nada
- P-40 Highly Sensitive Hydrogen Sulphide Gas and Methylene Blue Dye Sensors Based on Carboxymethyl Cellulose Sodium and CuO@ZnO Core/Shell: A DFT/TD-DFT Study
Rania Badry
- P-41 Molecular modeling and biological activities of metal oxide modified bioactive glass

Taha Taima

P-42 The effect of Mn content on CdS Nanoparticles: morphological and dielectric properties

Rasha S. Ibrahim

P-43 $Zn_{0.97-x}Cu_{0.03}V_xO$ ($x = 0, 0.02, 0.04$) microrods structures: Optical, refractive index, electrical and photocatalytic properties

Ahmed M. Youssef

P-44 Evaluation of the VITEK®2 Cards for Rapid Direct Identification and Antimicrobial Susceptibility Testing of Human Pathogenic Bacteria

Yasser A. El-Ameir

P-45 Spectroscopic studies and antibacterial activities of 11H-indeno [1,2-b] quinoxaline-11-one

Dalia S. Onsy

P-46 Antibacterial Effect of Myco-Synthesized Nano-Silver Against Multidrug Resistant Bacteria

Nada H. Ghazala

P-47 Methyl Blue Removal and Antibacterial Activity of Copper/Zinc Bimetallic Nanoparticles Synthesized by Fusarium Oxysporum

Mai Taha

P-48 Antibacterial Activity Using Eco-Friendly Synthesized Zinc Nanoparticles

Aya Aboelnga

P-49 Biotechnological Studies on Some Bacteria from Avocado Fruits

Nada Mansour

P-50 Biochemical Synthesis of Some Metal Nanoparticles Using Pulicaria Undulata Extracts and Evaluation of Their Antioxidant, Antimicrobial and Cytotoxic Activity

Balasm T. Abduljabbar