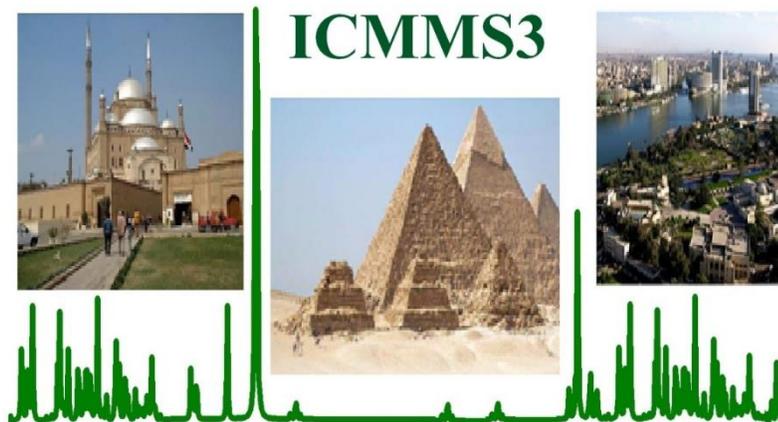


The Third Virtual International Conference on Molecular Modeling and Spectroscopy

15- 16September 2021, Cairo, Egypt



Under the Auspices of

Prof. Mohamed Hashem

President of the
National Research Centre, NRC

Prof. Gad El-Qady

President of the National Research
Institute of Astronomy and Geophysics,
NRIAG

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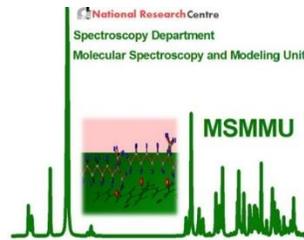
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Conference Program

First Day: Wednesday September 15, 2021

Time	Session	
10:00	S1: Opening Session	O-01 to O-06
11:00	S2: Keynote Lectures-1	KNL01 to KNL05
13:15	Open Discussion	
14:00	S3: Oral Session-1	O-07 to O-17
16:00	Open Discussion	
16:30	S4: Oral Session -2	Science Cafe
18:30	Open Discussion	
S5: Poster Session	P-01 to P-33	All Day in Science Café YouTube
19:00	Poster Open Discussion	

Second Day: Thursday September 16, 2021

Time	Session	
08:00	S6: Oral Session -3	O-18 to O-29
10:00	Open Discussion	
10:30	S7: Keynote Lectures-2	KNL06 to KNL10
13:00	Open Discussion	
14:00	S8: Oral Session-4	O-30 to O-40
16:00	Open Discussion	
16:30	S9: Oral Session-5	O-41 to O-50
17:00	Open Discussion	
17:30	Recommendations & Closing Ceremony	

List of Keynotes

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KNL-01	Application of Molecular Modeling and Spectroscopic Analyses in Cultural Heritage Medhat A. Ibrahim
KNL-02	Photoionization and Electron-Ion Recombination of Ca Ion Recombination of Ca Ions for Astrophysical Modeling Sultana N. Nahar
KNL-03	Physics of Galactic Winds: X-ray Diagnostics and the Acceleration of Cool Gas Todd A. Thompson
KNL-04	Investigating Model Lipid Membranes Complementarily by Raman and Neutron Scattering. Search for Raman Markers of NETosis. Grigory Arzumanyan
KNL-05	High Performance of Commercial Solar Cells Stacked by Crystalline p-n Silicon Nanowires Lotfia El Nadi
KNL-06	Predicting Conformational Changes in Riboswitch RNA upon Ligand Binding Fareed Aboul-ela
KNL-07	Green Economy and Wastes: How is it Possible to Combine Them? Paola Grenni
KNL-08	Innovation and Opportunities Toward New Molecules for The Agrochemical Industry: from Theory to Application Teodorico De Castro Ramalho
KNL-09	Novel Approaches on the Microextraction and Solid Phase Microextraction for Traces Species from Environmental Samples Mustafa Soylak
KNL-10	Structural Properties of Lipid Membranes: Experimental and Model Studies Kh.T. Kholmurodov

List of Orals

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O-01	Preface: Welcome Speech Prof. Medhat A. A. Ibrahim Conference Chairman
O-02	Preface Welcome Speech: The Third International Conference on Molecular Modeling and Spectroscopy Prof. Ahmed A. Fakhry Conference Honorary Chairman
O-03	Preface Welcome Speech: Welcome all of You in the Third International Conference on Molecular Modeling and Spectroscopy. Prof. Yehia Bahei El-Din

- O-04 Preface Welcome Speech: Welcome all of You in the Third International Conference on Molecular Modeling and Spectroscopy.
Prof. Mohamed M. Hashem
- O-05 Preface Welcome Speech: Welcome all of You in the Third International Conference on Molecular Modeling and Spectroscopy.
Prof. Gad El-Qady
- O-06 Preface Welcome Speech: Welcome all of You in the Third International Conference on Molecular Modeling and Spectroscopy.
Magdy Sabek
- O-07 Two-Dimensional Quantum Dots: Properties and Applications
Hazem Abdelsalam
- O-08 Application of Monte Carlo Method to Simulate Radiation Transfer Through Exoplanetary Atmospheres
Michael F. Rothman
- O-09 Electronic Properties and Molecular Electrostatic Potential Mapping of GQDs Decorated with ZnO, CuO, and TiO₂
Medhat A. Ibrahim
- O-10 Electronic and Physical Studies for Teflon FEP as a Thermal Control in Low Earth Orbit Reinforced with ZnO and SiO₂ Nanoparticles
Hend A. Ezzat
- O-11 Application of Carboxymethyl Cellulose Sodium/CuO Nanocomposites as a Sensor for NH₃ and H₂S Gases: Modeling Approach
Rania Badry
- O-12 Molecular Modeling Analysis of Chitosan-Dopamine Blend with Iron Oxide Nanoparticles for Tissue Engineering Applications
Nayera El-Sayed
- O-13 On the Analyses of Polytetrafluoroethylene Modified with Nano ZnO and SiO₂
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- O-14 DFT:B3LYP/LANL2DZ Study for Polyvinylchloride Enhanced with Metal Oxides/GQDs Applied as Anti-reflection Coating for Solar Cell
Hanan Elhaes
- O-15 Application of Modified Graphene as a Biosensor
Hanan A. T. Matar
- O-16 Modeling the Electronic Properties for CNT Interacted with ZnO, CuO and Co₃O₄
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- O-17 The Detection of NH₃, H₂S and HBr Gases by Carboxymethyl Cellulose Sodium/ZnO Nanocomposites: A Theoretical Study
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- O-18 Direct Binding of Small Heat Shock Protein α B-Crystallin and *Spike Protein* of SARS-CoV-2. Coarse-Grained Molecular Dynamics Simulations
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- O-19 Investigating the Dissociation Process and Binding Free Energy of p53-DBD/DNA Complex by PaCS-MD and MSM
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- O-22 Natural Nanofiber for Effective Treatment of Burn Wound
Sommaya M. Sharaf
- O-23 On the Applications of Biomaterials in Different Disciplines
Taha Taima
- O-24 Synthesis and Study of Mechanical Properties, Antibacterial Activity of GO, and PAA Containing Hydroxyapatite Nano Powder.
Taha Tiama
- O-25 Preparation and Characterization of Magnetic Thermoresponsive Nanocomposite for Hyperthermia and Drug Delivery Application
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- O-26 Nanofibrous ZnO/PVDF Filter Fabrication as a Potential Face Protector against Respiratory Viral Infections: Simulation and Experimental Studies
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Mixed-Ligand Complexes

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Safaa. R. Fouda
- O-48 Correlation between the Static Refractive Index and the Optical Bandgap: Review and New Empirical Approach
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- O-49 Simple Processed Polyvinyl Alcohol/Multi-Wall Carbon Nanotube Semi-Transparent Nanocomposites for High-Performance Optoelectronics
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P-04	Synthesis and Characterization of Chitosan Antimicrobial Containing Iron Oxide Nanoparticles Ahmed Farghaly
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P-06	Density Functional Theory, FTIR, UV-Vis Spectroscopic Studies of Cellulose Acetate Dimer and Cellulose Acetate Dimer /1, 2 MoO ₃ Dina Ezzat
P-07	Resent Spectroscopy Trends to Explain the Solar Neutrino Problem Magda M. Farghaly
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P-12	Effect of GQDs on Polytetrafluoroethylene/Metal Oxide Nanocomposite: Modeling Approach Medhat A. Ibrahim
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Science for the Society: Science Cafe

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SC-09	Working Principle and Sensing Mechanism of Metal Oxides Based Gas Sensors
SC-10	Simple Electronic Rain Alarm
SC-11	Evaluating the Humidity Sensor Behavior for MWCNTs Boosted with Co_3O_4 Nanorods
SC-12	Molecular Modeling for the Beginners
SC-13	Molecular Modeling using Electronic Structure Method
SC-14	Building Model Molecule for Starting Molecular Modeling Calculations
SC-15	My First Modeling Job: Optimization of Small Molecule
SC-16	My First Modeling Job: Vibrational Assignment
SC-17	My First Modeling Job: Polyvinyl Alcohol PVA
SC-18	My First Modeling Job: Graphene Quantum Dots GQDs
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SC-20	My First Modeling Job: Graphene Oxide/ Mn_2O_3 for Water Treatment
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SC-22	Application Example for QSAR Descriptors
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