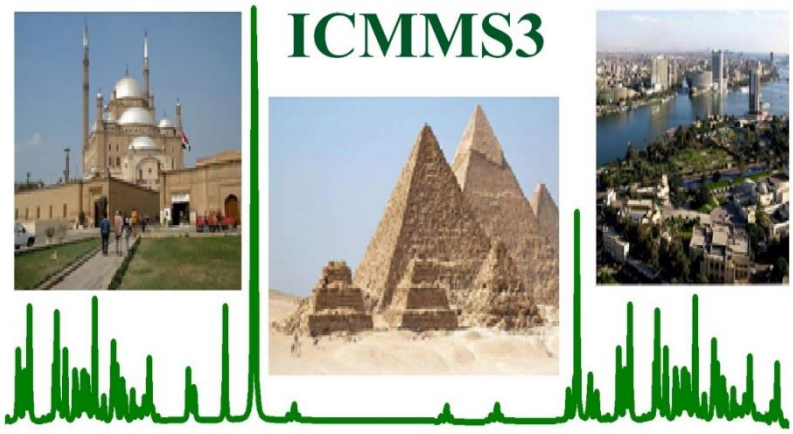
The Third Virtual International Conference on Molecular Modeling and Spectroscopy

15- 16September 2021, Cairo, Egypt



Under the Auspices of

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

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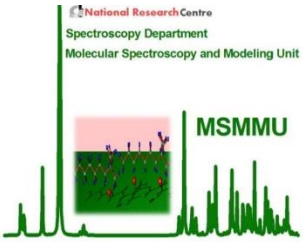

Conference Program

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

No	Title
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

No	Title
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-21 Nanomaterials for Biomedical Applications: Production, Characterizations, Recent Trends and Difficulties
Mostafa Mabrouk

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
Alaa AL Rahman Gamal

O-26 Nanofibrous ZnO/PVDF Filter Fabrication as a Potential Face Protector against Respiratory Viral Infections: Simulation and Experimental Studies
Hassan Nageh

O-27 Confocal Laser Scanning Microscopy and Qualitative Evaluation of Biological Samples
Heba ElSayed ElZorkany

O-28 Synthesis and Characterization of Nano CuO/ZnO/Al2O3 Catalyst via Laser Ablation Route for the Preparation of Some Cyanoacetanilide Derivatives
Ahmed Sarhan

O-29 The Influence of Additions of Molybdenum Trioxide Nanoparticle on the Structural and Optical Properties of Cellulose Acetate Film
Dina Ezzat

O-30 Spectroscopic Studies of Dy^{3+} Ion Doped Molybdenum Bismuth Borate Glasses for Optical Application
Amal Metwally

O-31 Adsorption Physiognomies of Methylene Blue Using Borate Bioactive Glass Ceramics Containing Silver Nanoparticles
Mohamed Abdelbaky

O-32 AC Conductivity and Dielectric Behaviour of Chitosan/Polypyrrole Blend
Nermin Gewili

O-33 Preparation and Characterization of Borosilicate Bioglass
Walaa M. Awad

O-34 NiFeCr Buffer and Capping Layer Impact on Exchange Bias and Planar Hall Effect Sensors Profile for NiFe/Au/IrMn Thin Films
Amir Elzwawy

O-35 Structural Study of Di-indium Tri-sulfuric (In_2S_3) Thin Films Fabricated by Sulfurization of Indium Thin Films using CVD Method
Ahmed I. Ali

O-36 The Effect of TiO_2 Nanoparticles on Varnish: Linear and Nonlinear Optical Properties
Ahmed I. Ali

O-37 Audio SIMO System Based on Visible Light Communication using Cavity LEDs
Mohamed Abdel-Hady

O-38 Synthesis, Potentiometric, Catalytic, Thermal and Biological Activity of Copper

Mixed-Ligand Complexes
Nelly H. Mahmoud

O-39 Microwave Assisted Synthesis of Co Doped SnO_2/rGO for Indoor Humidity Monitoring
Mohamed Morsy

O-40 Ultrafast Response Humidity Sensors Based on Polyvinyl Chloride/Graphene Oxide Nanocomposites for Intelligent Food Packaging
Mohamed Morsy

O-41 Hybrid Multifunctional TiO_2@g-C_3N_4 for Superior Visible-Photodegradation of Organic Dye and Pharmaceutical Compounds
Mai S.A. Hussien

O-42 Gamma-Ray Attenuation Properties of $Cu_2CdSn_3S_8$ and Binary Sulfide Compounds (Cu/Cd/Sn S) by using Phy-X/PSD Software
Nehal Sabry

O-43 Synthesis, Optical Properties, and Impedance Spectroscopy of Na_2TeO_3 Doped Polyvinyl Alcohol as Novel Polymeric Electrolyte Films
Mervat I. Mohammed

O-44 Structure, Magnetic and Photocatalysis of $La_{0.7}Sr_{0.3}MO_3$ (M=Mn, Co and Fe) Nanoparticle Perovskite: A Comparative Synthesized Route
Mohamed H. Ghozza

O-45 Discussions on the Film Design and Mechanical Properties of Y^{3+}/PVA Polymeric Composite Films: Enhancement of the Electrical Conductivity and Dielectric Properties
Fatma El-Sayed

O-46 Thickness Effect on Structural and Linear/Nonlinear Optical Properties of Acid Fuchsin Thin Films on FTO
Shenouda S. Shenouda

O-47 Magnesium Oxide-Anchored Graphene as a Swift Nanocatalyst for Degradation of 4-Aminophenol and Streptomycin
Safaa. R. Fouda

O-48 Correlation between the Static Refractive Index and the Optical Bandgap: Review and New Empirical Approach
Hosam M. Gomaa

O-49 Simple Processed Polyvinyl Alcohol/Multi-Wall Carbon Nanotube Semi-Transparent Nanocomposites for High-Performance Optoelectronics
Ahmed M. Ismail

O-50 Investigating the Structural Morphology, Linear/Nonlinear Optical Characteristics of Nd_2O_3 Doped PVA Polymeric Composite Films: Kramers-Kroning Approach
Tkrayte H. AlAbdulaal

List of Posters

No	Title
P-01	Electronic and Magnetic Properties of Graphene Quantum Dots Doped with Alkali Metals Hazem Abdelsalam
P-02	Two-Dimensional Si_2BN Nanoflakes for Efficient Removal of Heavy Metals Hazem Abdelsalam
P-03	Quantum Chemical Studies on Structural, Spectroscopic, Thermochemistry, Photo-Physical and Bioactivity Properties of m-Cresol Purple Dye Mohamed A.M. El-Mansy
P-04	Synthesis and Characterization of Chitosan Antimicrobial Containing Iron Oxide Nanoparticles Ahmed Farghaly
P-05	Influence of Annealing Temperatures on Nonlinear Optical, Dielectrical, Semiconducting Results and Fermi Level Position for $Cdp_{0.03}Te_{0.97}$ Thin Film Ahmed Abdel Moez
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
P-08	Application of Chitosan/Fe_3O_4 Nanocomposite as Biosensor Taha M. Tiama
P-09	Electronic Properties Study of Polyethylene Oxide/Metal Oxides Nanocomposite Reinforced with GQDs as Optoelectronic Application Maroof A. Hegazy
P-10	Theoretical Study of Polyvinyl Alcohol/Metal Oxides/GQDs Hybrid Nanocomposite as Humidity Sensor Medhat A. Ibrahim
P-11	Theoretical Study of Isomerization and Polymerization in Polyethylene Terephthalate Lobna A. Heikal
P-12	Effect of GQDs on Polytetrafluoroethylene/Metal Oxide Nanocomposite: Modeling Approach Medhat A. Ibrahim
P-13	Morphological Features, Structural Variation of Eco-Friendly Nancomposite of ZnO/TiO_2 Synthesized via *Hibiscus* Rosa-sinensis Extract Abdelrhman A. Menazea
P-14	Theoretical Spectroscopy Study of Dimers Kherfia Belabed and Mohamed A. Benmalti
P-15	Synthesis and Characterization of PVVH/CuO Nanoparticles to be used in Industrial Application Fatma Attia
P-16	Structural Peculiarities of Borate Bioglass Doped with Silver Oxide Eman.M. Abdallah

Rasha A. Youness

P-33 Calcium Phosphate Compounds as Successful Biomaterials for Bone Replacement Applications
Rasha A. Youness

Science for the Society: Science Cafe

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 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	Nano Club at Nanotechnology Research Center (NC-NTRC) The British University in Egypt, BUE
SC-06	Safety Rules and Guidelines for Working in Chemistry Laboratory
SC-07	Equipment's and Functions in Chemistry Laboratory
SC-08	How to Build up Handmade Electrospinning Technique?
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
SC-19	Molecular Modeling Study for Graphene Modified with Metal Oxides
SC-20	My First Modeling Job: Graphene Oxide/Mn_2O_3 for Water Treatment
SC-21	Introduction to QSAR Descriptors
SC-22	Application Example for QSAR Descriptors
SC-23	Removal of Atrazine from Contaminated Water by Graphene Quantum Dots
SC-24	Si_2BN Quantum Dots as an Efficient Detector of Carbamazepine in Aqueous Environment