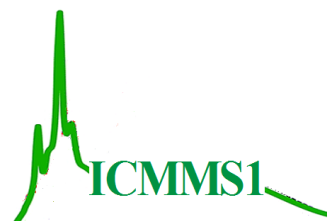


The First International Conference on Molecular Modeling and Spectroscopy

19-22 February 2019

National Research Centre, Cairo, Egypt



Program of the Conference

Tuesday February 19, 2019

New Hall, National Research Centre

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| 09:00-10:00 | Registrations |
| 09:30-10:30 | Opening Ceremony |
| | Prof. Medhat Ibrahim Conference Chairman OL-01: Preface: Welcome Speech |
| | OL-02: The First International Conference on Molecular Modeling and Spectroscopy Prof. Ahmed Fakhry |
| | OL-03: Welcome to the National Research Centre Prof. Mohamed Hashem President of the National Research Centre |
| | OL-04: In the Memory of Prof. Mohamed El-Okr Dr. Mohamed Saleh |
| 10:25-10:30 | Photo Session |
| 10:30-11:00 | Coffee Break |
| 11:00-13:00 | Plenary Session I: PSI |
| 11:00-11:15 | OL-05 Molecular Modeling and Molecular Spectroscopy at NRC Medhat Ibrahim |
| 11:15-11:35 | OL-06 Fluorescence of Dye Molecules by Laser Multiphoton Excitation to Image Biological Cells Lotfia El Nadi |
| 11:35-12:05 | OL-07 Novel Catalysts for Converting CO and CO₂ Pollutants to Added Value Hydrocarbon Products Ahmed Abd El-Moneim |
| 12:05-12:20 | OL-08 Microfluidics Devices for Biomedical Applications Amina Omar |
| 12:20-12:40 | OL-09 Molecular Dynamics: From Simple Liquid to Polymer Nanocomposites Fathia Mohamed |
| 12:40-13:00 | OL-10 Strategy of NLEBA for the mass production of nanomaterials for environmental and biomedical applications Ibrahim S. Yahia |
| 13:00-13:15 | O-35 Molecular Modeling in Drug Discovery: A shortcut to Identify Molecular Targets and Bioavailability of Biological Lead Compounds Ahmed Atef Ahmed Ali |
| 13:15-13:30 | OL-11: Modeling and Spectroscopic Analyses of Coptic Icons Ahmed Refaat |
| 13:30-13:45 | O-36 Tuning the Plasmon/Exciton Coupling in Different Regimes for |

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| | Tailoring the Shapes of the Metal and Semiconductor Nanocomposites A. Okasha |
| 13:45-14:00 | O-37 Protein Dynamics on Single Molecule Level with Fluorescence Correlation Spectroscopy D. Atta |
| 14:00-14:05 | Discussion |
| 14:05-15:00 | Lunch |
| 15:00-17:30 | Science for the Society: Science Café: SC Osc-20-Osc-34 |
| 15:00-17:30 | Plenary Session II: PSII (Hall D) |
| 15:00-15:10 | O-38: Ultrasonic Assisted Photocatalytic Degradation of Ciprofloxacin using Bimetallic Nanoparticles R. O ZamanBrohi |
| 15:10-15:20 | O-39: Modeling the Mechanism of Iron Oxide/TiO₂ /PVA Nanocomposite for Removal of Heavy Metals. Y. Abdulhady |
| 15:20-15:30 | O-40: Modeling and Spectroscopic Analyses for Nano Modified Chitosan as Biosensor N. S. Alghunaim |
| 15:30-15:40 | O-41: Biosorption of Zinc(II) and Cadmium(II) Using Ziziphus Spina Stones E. A. Assirey |
| 15:40-15:50 | O-42: Molecular Modeling Evaluation of Silicon/Polyaniline/ZnO Nanocomposite N. S. Alghunaim |
| 15:50-16:00 | O-43: Computational study for the complexation of hydrated lead and 1,3,4-Thiadiazole-2,5-dithiol E. Yalmaz |
| 16:00-16:10 | O-44: Effect of Hydration on the Electronic Properties of Si/PANi/3ZnO Nanocomposite N. S. Alghunaim |
| 16:10-16:20 | O-45: On the Effect of Pollutants on the Molecular Structure of Fish Z. Al-Fifi |
| 16:20-16:30 | O-46: Novel composite for lead ions removal from wastewater E. A. Assirey |
| 16:30-16:45 | Discussion |
| 15:00-17:30 | Poster Session I: P1-P44 (Hall E) |

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| 08:30-09:30 | Plenary Session III: PLIII |
| 08:30-08:40 | O-47: Molecular Modeling Study for the Chitosan Ibuprofen Interaction A. M. Bayoumy |
| 08:40-08:50 | O-48: Removal of Ibuprofen Using Chitosan Biopolymer: Theoretical and Experimental Studies A. M. Bayoumy |
| 08:50-09:00 | O-49: Polymer Electrolytes Based on Plasticized Sodium Carboxymethyl Cellulose Doped with Acetic Acid R. Badry |
| 09:00-09:10 | O-50: Optimizing the Electrospun Parameters which Affect the Preparation of Nanofibers A. Fahmy |
| 09:10-09:20 | O-51: On the Molecular Modeling Analyses of Sodium Carboxymethyl Cellulose Doped with Acetic Acid R. Badry |
| 09:20-09:30 | O-52: Effect of Nano Metal Oxides on the Electronic Properties of Cellulose, Chitosan and Sodium Alginate H. A. Ezzat |
| 09:30-10:10 | OL-12: Polarization-sensitive CARS Imaging and Surface-Enhanced Micro-CARS of Organic Molecules Grigory Arzumanyan |
| 10:10-10:40 | Coffee Break |
| 10:40-13:55 | Plenary Session IV: PLIV |
| 10:40-11:20 | OL-13: Pre-Colombian Art – Old, New, Fakes: Experimental approaches Wolfram Baumann |
| 11:20-12:00 | OL-14: The Experimental and Molecular Dynamics Studies of the DNA Radiation Damage and Conformation Behavior on a Zirconium Dioxide Surface Kholmirzo Kholmurodov |
| 12:00-12:30 | OL-15: Model of Collagen Structures Mineralization Sylwia Orzechowska |
| 12:30-13:10 | OL-16: Quantum Dots in Molecular Diagnosis Pavel Gladyshev |
| 13:10-13:20 | O-53: The DFT Study of the Electronic and Optical Properties of Functional Materials M. Subhoni |

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| 13:20-13:35 | O-54: Quantum-chemical Calculations of Lead-Free Perovskite Materials on the Basis of the Density Functional Theory K. Rahmonov |
| 13:35-13:45 | O-55: Modeling the Effect of Metal Substitution on the Electronic Properties of Fullerene and Fullerypyrrolidine H. Elhaes |
| 13:45-13:55 | O-56: Molecular Spectroscopic Study of Dried Water Hyacinth M. Ibrahim |
| 14:00-14:30 | Lunch |
| 14:30-18:00 | Poster Session II: P44-P88 |
| 14:30-17:00 | Plenary Session V: PSV |
| 14:30-15:10 | OL-17: The New Generation Green Solvents for the Spectroscopic Determinations of Trace Metals Mustafa Soylak |
| 15:10-15:20 | O-57: Spectroscopic Study of Heavy Metals Interaction with Organic Acid M. Abd El-Aal |
| 15:20-15:30 | O-58: Portable and Battery Operated Highly Sensitive Ammonia Gas Sensor Based on CNTs/rGO/ZnO Nanocomposite M. Morsy |
| 15:30-15:40 | O-59: Separation, Preconcentration and Determination of BrilliantBlackBN in food samples by using microextraction-UV-Vis spectrophotometry M. Soylak |
| 15:40-15:50 | O-60: Visible photocatalytic nanomaterials for Wastewater Treatments M. S.A. Hussien |
| 15:50-16:00 | O-61: Molecular Modeling Analyses of the Effect of Nano Metal Oxides on Heme Molecule O. Osman |
| 16:00-16:10 | O-62: Mesoporous CNTs/Co₃O₄@rGO Nanocomposite as sensor for Volatile Organic Compounds M. Morsy |
| 16:10-16:30 | O-63: Removal of Hydrated Heavy Metals by Graphene Quantum Dots H. Abdelsalam |
| 16:30-16:40 | O-64: Cost Effective Sensor Based on SnO₂ Modified with CNTs and Graphene M. Morsy |
| 16:40-16:50 | O-65: Structural, Optical, Morphological and Thermal Properties of Nanocomposite Based on Poly (ethylene-co-vinyl alcohol) Filled with Graphene Oxide A. Y. Yassin |
| 16:50-17:00 | O-66: Enhancement of Spectroscopic, Thermal, Electrical, Dielectric and Morphological Properties of Polyethylene Oxide/Carboxymethyl |

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| | Cellulose Blends: Combined FTIR/DFT M. A. Morsi |
| 17:00-17:10 | O-67: Molecular Spectroscopic Analysis of Sodium Phosphate Zinc Copper Doped Magnesium Glass Matrix Y. H. Elbashar |
| 17:10-17:20 | O-68: On the Analyses of Cellulose and Chitosan: Spectroscopic and Modeling Approach A-A. Mahmoud |
| 17:20-17:30 | O-69: Reactivity of some Functional Groups: Modeling Approach A-A. Mahmoud |
| 17:30-17:40 | O-70: Ab initio Molecular Modeling Analysis of Dioxin O. Osman |

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| 08:30-09:30 | Plenary Session VI: PSVI |
| 08:30-08:40 | O-71: Effect of Ultraviolet Radiation on Original Activity Remaining of <i>Spodoptera littoralis</i> Nuclear Polyhedrosis Virus Against <i>Spodoptera littoralis</i> Boisd (Lepidoptera: Noctuidae) S. M. M. Abd EL-Aziz |
| 08:40-08:50 | O-72: Green Route for the Removal of Pb from Aquatic Environment A. Refaat |
| 08:50-09:00 | O-73: Synergetic Behavior of Gamma-Irradiated Modified Borate Bioglass Analogous to Hench's Bioglass A. Okasha |
| 09:00-09:40 | OL-18: Study for a Clue of Extra-Terrestrial Life: Phosphorus Sultana N. Nahar |
| 09:40-09:55 | O-74: Molecular Modeling, In Vitro Bioactivity Assessment and Mechanical Properties of some Phosphate Glasses R. A. Youness |
| 09:55-10:10 | O-75: Modified Chitosan Blends as Biosensor for Amino Acids A. Refaat |
| 10:10-10:40 | Coffee Break |
| 10:40-12:40 | Plenary Session VII: PSVII |
| 10:40-11:20 | OL-19: Tunable Plasmonics in Graphene for Energy Biotechnology Applications Amal Kasry |
| 11:20-11:35 | O-76: Preparation and Characterization of Chitosan/Calcium Phosphate Fiber for Biomedical Application A. Omar |

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| 12:35-12:50 | O-77: On the Molecular Modelling Structure of the Egyptian Soil/Sediment in River Nile Delta Region H. Elhaes |
| 12:50-13:05 | O-78: Biophysical Properties and Molecular Modeling Study of Collagen Blends for Possible Application as Meshes for Hernia Repair A. Refaat |
| 13:05-13:20 | O-79: The Influence of Sintering Temperatures on the Molecular Structure, Physical and Mechanical Properties of Zirconia/Hydroxyapatite Nanobiocomposites R. A. Youness |
| 13:15-13:30 | O-80: Radiometric and Instrumental Neutron Activation Analysis Investigation of Radioactive ^{137}Cs and ^{210}Pb as well as some Major and Trace Elements in Lacustrine and Euxinic Unconsolidated Sediments of Danube Delta and Western Black Sea Shore O. G. Dului |
| 13:30-13:45 | O-81: Fullerene and its hydroxylated nanoparticles – human γD-crystallin interaction explained by in silico approach A. A. Gawad |
| 13:45-14:30 | Lunch |
| 14:30-16:00 | Plenary Session VIII: PSVIII |
| 14:30-14:45 | O-82: Constructive Coupling between BiFeO_3 and CoFe_2O_4; Promising Magnetic and Dielectric Properties N. G. Imam |
| 14:45-14:55 | O-83: Photoacoustic Study of Optical and Thermal Properties of Cu_2S Quantum Dots Sensitized Solar Cell Photoanode A. Khalid |
| 14:55-15:05 | O-84: Improving the Efficiency of QDSSCs Based on $\text{TiO}_2/\text{CdS}(\text{Silar})/\text{TBAI}$ Capped CdSe (Colloid) Photoanodes. M. Nabil |
| 15:05-15:15 | O-85: Effect of of CdS Quantum Dots Size on Thermal and Photovoltaic Parameters of Quantum Dots Sensitized Solar Cells (QDSSCs) A. Khalid |
| 15:15-15:25 | O-86: Size Effect of TBAI Capped CdSe Nanoparticles on the Quantum Dots Sensitized Solar Cells M. Nabil |
| 15:30-16:30 | Closing Ceremony Recommendations |

OL: Keynote Lecture

O: Oral

P: Poster