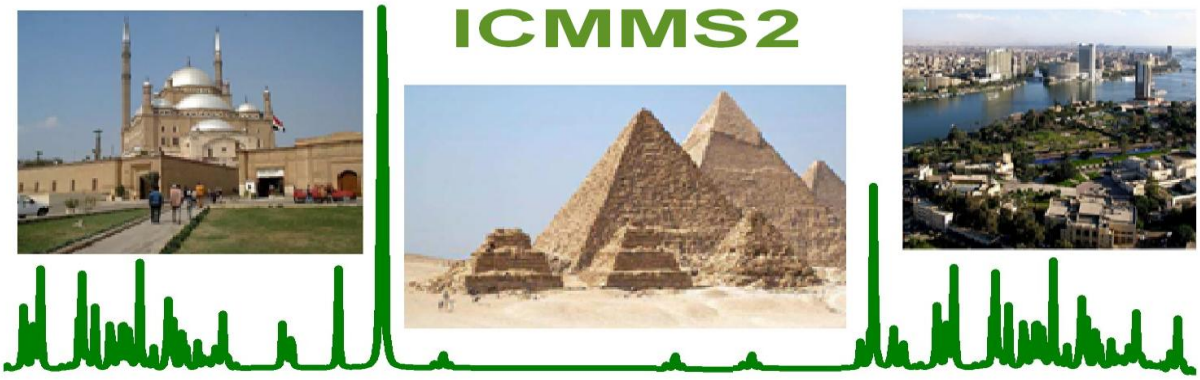
المؤتمر الدولي الثاني للاطياف والنمذجة الجزيئية
23- 24 سبنمبر 2020
المركز القومي للبحوث - القاهرة - مصر



تحت رعايه

الأستاذ الدكتور/محمد محمود هاشم

رئيس المركز القومي للبحوث

الرئيس الفخري للمؤتمر

الأستاذ الدكتور/أحمد عبدالرحمن فخري

رئيس المؤتمر

الأستاذ الدكتور/مدحت ابراهيم

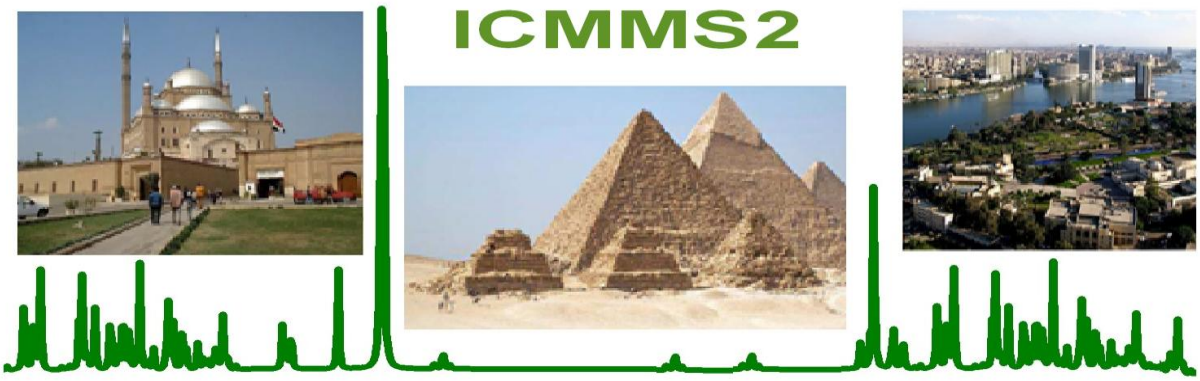
نائبا رئيس المؤتمر

الأستاذ الدكتور/أسامه عثمان و الأستاذ الدكتور/حنان الحايس

سكرتيرة المؤتمر

د. هند عزت

The Second International Conference on Molecular Modeling and Spectroscopy
23-24 September, 2020
National Research Centre, Cairo, Egypt



Under the Auspices of

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Short Program

First Day: Wednesday September 23, 2020

Time	Session	
09:00	**S1: Opening Session**	O-01 – O-03
09:30	**S2: Keynote Lectures-1**	KNL01 – KNL06
	Open Discussion	
10:00	**S3: Poster Session-1**	P01- P20
12:00	**S4: Oral Session-1**	O-04 – O-14
	Open Discussion	
14:30	**S5: Oral Session -2**	O-15 – O-22
	Open Discussion	
17:00	End of Poster Session and Open Discussion	

Second Day: Thursday September 24, 2020

Time	Session	
09:00	S6: Keynote Lectures-2	KNL07 – KNL14
	Open Discussion	
10.00	**S7: Poster Session-2**	P21- P39
12:00	**S8: Oral Session -3**	O-23 – O-33
	Open Discussion	
14:00	**S9: Oral Session-4**	O-34 – O-41
	Open Discussion	
16:30	**End of Poster Session and Open Discussion**	
	Best Paper Award & Best Poster Award & Young Researcher Award	
17:30	**Recommendations & Closing Ceremony**	

Conference activities will be through the following links:
The Science Café YouTube channel:
https://www.youtube.com/channel/UC7au-3_dZMX6BgRqLHDEBfQ

The modeling and simulation Facebook page
https://www.facebook.com/groups/728916337268494/

List of Keynotes

No	Title
KNL-01	Fabrication, Characterization of new Nanohybride Materials for Solid Phase Extraction of Trace Species Mustafa Soylak
KNL-02	Acknowledgments for Prof. Mustafa Soylak
KNL-03	Molecular Modeling and Molecular Spectroscopy at National Research Centre Medhat Ibrahim
KNL-04	The Perturbed Free Energy Landscape: Linking Ligand Binding to RNA Folding Fareed Aboul-ela
KNL-05	Single-Molecule Imaging by Surface-Enhanced Raman Spectroscopy Grigory Arzumanyan
KNL-06	Review of Solar Pumped Lasers Lotfia M. El Nadi
KNL-07	Contribution of Molecular Modeling and Spectroscopy to the Development of Methods for Proteomic Diagnostics of Coronavirus Diseases Gladyshev P. Pavel
KNL-08	The Study of Natural Microbial Community as a Tool for Assessing the Recovery of Polluted Environments. Grenni Paola
KNL-09	Recent Progress in Ultrafast Lasers and Laser Spectroscopy and its Environmental Applications Walid Tawfik
KNL-10	Molecular Dynamics Simulations of Lipid Membranes: the Cation-zwitterionic Lipid Interactions are Governed by the Lateral Area per Lipid Kholmirzo Kholmurodov
KNL-11	Ecology and Society. Impacted Ecosystems Marina Frontasyeva
KNL-12	Concordant Electron Paramagnetic Resonance and Thermoluminescence Age of a Romanian Plane Loess Deposit Octavian G. Duliu
KNL-13	Spectra of Phosphorus for Astrophysical Modeling Sultana N. Nahar
KNL-14:	Overview of Sol - Gel Advanced Nano-structure Material Applications Inas Kamal Battisha

List of Orals

No	Title
O-01	Preface: Welcome Speech Medhat A. A. Ibrahim Conference Chairman
O-02	The Second International Conference on Molecular Modeling and Spectroscopy

Ahmed A. Fakhry
Conference Honorary Chairman

O-03 Welcome in the Second International Conference on Molecular Modeling and Spectroscopy
Prof. Mohamed M. Hashem
President of National Research Centre

O-04 Removal of Pharmaceuticals from Aquatic Environment using Modified Biomaterials
Ahmed M. Bayoumy

O-05 Application of Natural Polymers Enhanced with ZnO and CuO as Humidity Sensor
Hend A. Ezzat

O-06 Optical, Conductivity and Dielectric Properties of Plasticized Solid polymer Electrolytes Based on Blends of Carboxymethyl Cellulose Sodium and Polyethylene Oxide
Rania Badry

O-07 Molecular Interactions of Fullerene-Based Derivatives and SARS-CoV-2
Alaa El-Din A. Gawad

O-08 Study of the Electronic Properties of Solid Polymer Electrolytes Based on Blends of CMC, PEO and Acetic acid
Hanan Elhaes

O-09 Physical and biophysical Analyses of Polyvinyl Alcohol/ Sodium Alginate/ZnO Composite
Ahmed Fahmy

O-10 Computational Notes on the Chemical Stability of Flutamide
Alaa El-Din A. Gawad

O-11 Dielectric Relaxation Behavior and AC Electrical Conductivity of Cellulose Acetate-Mollybdenum Trioxide Nanoparticle Blended Film
Dina Ezzat

O-12 Effect of Substitutions on the Electronic Properties of Acetylsalicylic Acid
Yasmine O. Osman

O-13 A combination of Analytical Methods to Evaluate the Effect of Humidity Aging on the Painting Materials of Icon Models
Mina Magdy

O-14 Electronic Properties of Polyvinyl Alcohol/ TiO_2/SiO_2 Nanocomposites
Fatma Gamal

O-15 Molecular Dynamics Simulations of the Alcohol Dehydrogenase Enzyme:
The Solvent pH Influence on the Protein Conformation Behavior
Ivan Andreyevich Baigunov

O-16 First Principles Calculations of Geometrical Structure and Electronic and Optical Properties of Brom-Doped $CsSnI_3$ Perovskite for Photoelectric Applications
Dilshod Nematov

O-17 Investigation of the Optical and Photoelectronic Properties of Quantum Dots for Immunochemical Analysis
Novikova Sagila

O-18 The use of Quantum Dots as Fluorescent Labels in the Immunochemical Method of Analysis
Novikova Sagila

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Gribova Elena

O-20 Hybrid Perovskite $CH_3NH_3PbI_3$ Bulk Crystals Synthesis by Temperature Lowering Method
Vladislav Kinev

O-21 The use of Multivariate Data Analysis Methods for the Selection of Promising Heat Storage Materials Based on Hydrate Salts.
Testov Dmitry Sergevich

O-22 Novel Bimetallic Nano Particles for Sorption of Mercury (II) from Drinking Water: Adsorption Experiment and Computational Studies
Rafi O Zaman Brohi

O-23 Treatment of Breast Cancer using Photothermal Therapy Induced by laser-Activated Gold Nanoparticles
Hend Gamal

O-24 Assessment of Heavy Metals Content in the Agricultural Soils of Kafr El-Zayat City using Laser Ablation Inductively Coupled Plasma Mass Spectroscopy (LA-ICP-MS) and Inductively Coupled Plasma Optical Emission Spectroscopy (ICP-OES)
Asmaa F. Mankoula

O-25 Determination of Electron Temperature of Cu I Lines 515.32, 521.82, and 522.0 nm using Ultrafast-LIBS
Walid Tawfik

O-26 Physical and Electrical Characterization of PVP/PVA Matrix Doped by Gold Nanoparticles Prepared by Laser Ablation
Abdelrhman A. Menazea

O-27 Alumina Surface Modified with Hydroxyapatite Sputtered via Pulsed Laser Deposition Technique for Biomedical Applications
Mohamed Afifi

O-28 Core-Shell of Au@Se |Nanoparticles Incorporated via Laser Ablation Technique into the Polymeric Nanofibrous Scaffolds of Cellulose Acetate/PVDF for Wound Healing Applications
Mohamed K. Ahmed

O-29 Nanosecond Laser Assisted the Improvement of the Structural, Optical and Electrical Properties of Carboxymethyl Cellulose/ Polyvinyl Alcohol Blend Filled with Biosynthesized Gold Nanoparticles
Mohamed Morsi

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Ayman M. Mostafa

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Olfat El-sayed

O-35 Zinc Oxide Nano-Rods: Challenges for Glucose Biosensors.
Hanan Abd El-Wahab

O-36 Kinetic Studies of Unimolecular Thermal degradation of Isopropyl Esters as Biofuel Surrogates: DFT and Ab Initio Studies
Lobna A. Heikal

O-37 Dielectric, Structural and Optical Properties of Nd^{3+} Ions Doped Phosphate Glasses
Mahmoud Ismail

O-38 Metal−Organic Frameworks for Hydrogen Storage and Carbon Capture: Theoretical Prospective
Lobna A. Heikal

O-39 Effect of the Implantation Biogenic Hydroxyapatite-Coated Ti/Al Alloy on the Wound Healing in Dogs
E.M. Mahmoud, M. Sayed, M. Awaad, M. Blum, A. Killinger, R. Gadow, Ashraf M. Abu-Seida, S.M. Naga.

O-40 Singlet Oxygen Generation by Nanocomposites Based on Quantum dots and Porphyrin in Chitosan Solution
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O-41 Antifouling PES/Cu@Fe_3O_4 Mixed Matrix Membranes: Quantitative Structure-Activity Relationship (QSAR) Modeling and Waste Water Treatment Potentiality
Ahmed Abdel-Karim

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P-03	Semiemperical Molecular Modeling Analyses for Graphene/Nickel Oxide Nanocomposite Islam Gomaa
P-04	Molecular Modeling Applied For Carbon Nano Materials Osama Osman
P-05	Application of Polyvinyl alcohol/Polypropylene/Zinc Oxide Nanocomposites as Sensor: Modeling Approach Ahmed Fahmy
P-06	Computational Notes on The Effect of (Li-Na-K) on Calcium Zinc Phosphate Oxide Glasses Hanan Elhaes
P-07	Molecular Modeling Analyses for Electronic Properties of CNT/TiO_2 Nanocomposites

Hanan Elhaes

P-08 Quantum Chemical Studies on Structural, Spectroscopic, Thermochemistry, Photo-physical and bioactivity properties of m-cresol purple dye
Mohamed A.M. El-Mansy

P-09 FT-IR, Molecular structure and nonlinear optical properties of 2-(pyranoquinolin-4-yl)malononitrile (PQMN): A DFT approach
Sara M. Atef

P-10 Modeling the Effect of Hydration on the Electronic and Vibrational Properties of AZT
Nayera El-Sayed

P-11 Computational Notes on the Molecular Modeling Analyses of Flutamide
Abdel Aziz Mahmoud

P-12 DFT:B3LYP/ LANL2DZ Study for the Removal of Fe, Ni, Cu, As, Cd and Pb with Chitosan
Aya A. Mohamed

P-13 Mapping Molecular Electrostatic Potential (MESP) for Fulleropyrrolidine and its Derivatives
Ahmed M. Bayoumy

P-14 Chitosan/Graphene Oxide Composite as an Effective Removal of Ni, Cu, As, Cd and Pb from Wastewater
Samah A. Ibrahim

P-15 Study of the Electronic Properties of Graphene Oxide/(PANi/Teflon)
Sara H. Radwan

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Mohamed S. Abdel-Aal

P-17 Theoretical investigation of hydrogen bonding between Adrenaline and hydrogen sulfide complexes utilizing DFT/□B97XD/6-311G basis's set
Amr Mohamed

P-18 Steglich Esterification and Computational study of alkyl propiolate derivatives
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P-19 Molecular Modeling Analyses for Modified Biopolymers
Amina Omar

P-20 Molecular Modeling Analyses for Polypropylene/Zinc Oxide Nanocomposite
Dina Shehata

P-21 Effect of Molybdenum Trioxide Nanoparticle Additions on the Structural and Optical Properties of Cellulose Acetate Film
Dina Ezzat

P-22 Molecular properties of polyvinyl alcohol/ sodium alginate composite
Ahmed Fahmy

P-23 Green technology for metal removal from contaminated water
Paola Grenni

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Hend A. Ezzat

P-25 Theoretical study of the cyclo-addition reaction
Kherfia.Belabed

P-26 First principles investigation of electronic properties of graphene doped with Al and