MES 2024 - International Conference on Molecular Electronic Structure

Saturday, September 21st

16:30 **Registration**

18:15 **Opening of the Conference**

18:30 **Keynote Lecture:** **Anna Krylov** (University of Southern California, USA)
Molecular Orbitals: Physical Reality or Mathematical Construct?

19:30 ***Welcome reception***

Sunday, September 22nd

SESSION 1 – Chair: Kasia Pernal

8:40 **Chemistry Europe Publishing Lecture IO1:**
Roland Lindh (Uppsala University, Sweden)
Variations on the use of subspace Gradient Enhance Kriging for SCF/DFT orbital optimization.

9:15 **IO2:** **Jiali Gao** (Shenzhen Bay Laboratory, China)
Multistate Density Functional Theory and Applications.

9:45 **IO3:** **Ireneusz Grabowski** (Nicolaus Copernicus University, Poland)
An evaluation of the Hybrid KS DFT Functionals based on the KS exchange-correlation potentials.

10:15 **CO1:** **Yangyi Lu** (Shenzhen Bay Laboratory, China)
Exact Properties of Multi-State Density Functional Theory.

10:35 **CO2:** **Renu Bala** (Nicolaus Copernicus University, Poland)
Theoretical study of spectroscopic constants and vibrational parameters for the ground state of AlX^+ (X: F, Cl, Br) ions.

10:50 ***Coffee Break***

SESSION 2 – Chair: Raffaele Resta

11:10 **IO4:** **Alex J. W. Thom** (University of Cambridge, United Kingdom)
Holomorphic Hartree-Fock and Density Functional Theories: A basis for multireference electronic structure?

11:40 **IO5:** **Sarai D. Folkestad** (Norwegian University of Science and Technology, Norway)
A spin-adapted coupled cluster model for open-shell molecules: core excitations in ionized molecules.

12:10 **CO3:** **Fahri Alkan** (Bilkent University of Ankara, Turkey)
TDDFT+TB Investigation of the Optical Properties of Metal Nanoclusters.

12:30 **F1:** **Alberto Barlini** (Scuola Normale Superiore Pisa, Italy)
Theory of magnetic properties in QED environments: application to molecular aromaticity.

12:40 **End of the session**

12:55 ***Lunch***

SESSION 3 – Chair: Peter Gill

14:45 **IO6:** **Joonho Lee** (Harvard University, USA)
Recent Progress in Auxiliary-Field Quantum Monte Carlo

15:15 **IO7:** **Viktor N. Staroverov** (The University of Western Ontario, Canada)
Are exchange-correlation potentials discontinuous at atomic nuclei in molecules?

15:45 **IO8:** **Kasia Pernal** (Łódź University of Technology, Poland)
On-top pair density functionals for wavefunction theories.

16:15 **F2:** **Anthuan Ferino-Pérez** (KU Leuven, Belgium)
Ab Initio computation of nonradiative decay with complex-variable methods

16:25 ***Coffee Break***

SESSION 4 – Chair: Josep Maria Bofill

16:45 **IO9:** **David P. Tew** (University of Oxford, United Kingdom)
Dynamic correlation for configuration state functions.

17:15 **IO10:** **Arnaud Leclerc** (Université de Lorraine, France)
Optimized complex Gaussian representation of electronic continuum states: application to molecular ionization processes.

17:45 **IO11:** **Niyazi Bulut** (Firat University, Turkey)
Mechanistic Exploration of Metal-Cation Interactions: Ab Initio Study of Mg/Al/NaC6H$^+$ Complexes.

18:10 **CO4:** **Jun Yasui** (Kwansei Gakuin University, Japan)
Progress in the study of algebraic molecular orbital equation.

18:25 **F3:** **Stéphanie Egome Nana** (Université de Lorraine, France)
Complex Gaussian-Type Orbitals expansion for the two-center continuum states.

18:35 **End of the session**

19:30 ***Dinner***

20:30 **POSTER SESSION**

Monday, September 23rd

SESSION 5 ***Frank Harris Memorial Session*** **– Chair: Philip Hoggan**

8:30 **IO12:** **Hendrik J. Monkhorst** (University of Florida, USA)
The Molecular Coupled-Cluster Method — A Solution in Search of Problems

9:00 **IO13:** **Peter Gill** (University of Sydney, Australia)
Minimal-basis Hartree-Fock calculations using the HILO approximation.

9:30 **IO14:** **Avram Sidi** (Technion - Israel Institute of Technology, Israel)
Spectrally accurate numerical quadrature formulas for periodic Hadamard Finite - Part integrals via Euler–Maclaurin expansions

10:00 **IO15:** **Harris J. Silverstone** (Johns Hopkins University, USA)
A Generalization of Padé Approximants with Application to Molecular Electronic Structure: Educated Match.

10:20 **CO5:** **James Avery** (University of Copenhagen, Denmark)
Folding Carbon: A Calculus for Molecular Origami.

10:35 ***Coffee break***

SESSION 6 – Chair: Anna Krylov

11:00 **IO16:** **Ksenia Bravaya** (Boston University, USA)
Electronic structure methods for shape and Feshbach resonances.

11:30 **IO17:** **Monika Musial** (University of Silesia in Katowice, Poland)
Fock space multireference coupled cluster method in the three-valence sector for description of electronic states of atoms and molecules

12:00 **IO18:** **Giovanni Bistoni** (Università degli Studi di Perugia, Italy)
Combining High Accuracy and Chemical Insights with Local Coupled Cluster Methods.

12:30 **CO6:** **Tommaso Nottoli** (Università di Pisa, Italy)
An Efficient Implementation of Coupled Cluster with Cholesky Decomposition and Point-group Symmetry.

12:45 **F4:** **Piotr Michalak** (University of Warsaw, Poland)
Rank-reduced equation-of-motion coupled cluster triples: an accurate and affordable way of obtaining excitation energies of molecules.

12:55 ***Lunch***

SESSION 7 – Chair: Ksenia Bravaya

14:10 **IO19:** **Andre Gomes** (Université de Lille, France)
Ground and excited state properties of heavy (and not so heavy) element systems from relativistic (embedded) coupled cluster calculations.

14:40 **IO20:** **Guillaume Thiam** (Università degli Studi di Perugia, Italy)
Toward a relativistic ab-initio methodology for strong photon-molecule interaction.

15:05 **CO7:** **Aleksandra Kyuberis** (University of Groningen, Netherlands)
Relativistic basis sets for SHE 119-122.

15:20 ***Coffee break***

SESSION 8 – Chair: Viktor Staroverov

15:40 **IO21:** **Tomasz Wesolowski** (Université de Genève, Switzerland)

Bottom-up strategy to approximate the bi-functional of non-additive kinetic potential for multi-level simulations of electronic structure in condensed phase.

16:10 **CO8:** **Federico Lazzari** (Scuola Normale Superiore, Italy)
From Semi-Experimental to Fully Theoretical Building Blocks of Large Molecular Systems: A Composite Approach to Equilibrium Geometry.

16:25 **CO9:** **Hela Ladjimi** (University of Warsaw, Poland)
Electronic structure and theoretical prediction of the formation of cold $BaAlk^+$ (Alk= Na, K, Rb, Cs) molecular ion.

16:40 **End of the session**

Tuesday, September 24th

8:30 **Greetings from the Rector of the University of Chieti-Pescara**

SESSION 9 – Chair: Shirin Faraji

8:45 **IO22:** **Markus Meuwly** (University of Basel, Switzerland)
Machine Learning-Based Potential Energy Surfaces with Applications to Spectroscopy and Chemical Reactions.

9:15 **IO23:** **Gábor Czakó** (University of Szeged, Hungary)
Automated ab initio potential energy surface developments for reaction dynamics computations.

9:45 **IO24:** **Riccardo Conte** (Università degli Studi di Milano, Italy)
Building accurate and efficient ab initio potential energy surfaces for vibrational spectroscopy calculations via permutationally invariant polynomials.

10:15 **CO10:** **Shmuel Zilberg** (Ariel University, Israel)
Light-driven photoswitches: molecular system leading to single photoproduct via Conical Intersection, and exothermic reverse reaction.

10:35 **CO11:** **Valter H. Carvalho-Silva** (Goiás State University, Brazil)
Kinetics of Rate Processes from Micro to Meso, Towards Macro - A Journey from Physicochemical Processes to Environmental Complexity.

10:55 ***Coffee break***

SESSION 10 – Chair: Seiichiro Ten-no

11:15 **IO25:** **Thomas Jagau** (KU Leuven, Belgium)
Recent progress about quantum chemistry for electronic resonances.

11:45 **IO26:** **Filippo Lipparini** (Università di Pisa, Italy)
An efficient and robust implementation of CASSCF linear response theory.

12:15 **IO27:** **Hilke Bahmann** (Bergische Universität Wuppertal, Germany)
Electronic structure at molecule-semiconductor interfaces.

12:45 **F5:** **Ritaj Tyagi** (Tata Institute of Fundamental Research, India)
Efficient Electron Affinity Predictions Using the Single-Pole Polarization Model.

12:55 ***Lunch***

SESSION 11 – Chair: Lichang Wang

14:15 **CO12:** **Massimiliano Bartolomei** (Instituto de Física Fundamental, Spain)
Cationic copper clusters in molecular hydrogen: solvation structures and bonding.

14:35 **CO13:** **Carlos Cárdenas** (Universidad de Chile, Chile)
Floquet Engineering of Molecules through a Bichromatic Radiation Field.

14:55 **CO14:** **Hamilton B. Napolitano** (Universidade Estadual de Goiás, Brazil)
Aqueous solubility of diclofenac diethylammonium: a molecular modeling study in solid state and solvation processes.

15:10 **End of the session**

15:30 ***Excursion***

Wednesday, September 25th

SESSION 12 – Chair: Roland Lindh

8:30 **IO28:** **Shirin Faraji** (Heinrich Heine University Düsseldorf, Germany)
Databased accelerated on-the-fly hybrid quantum/classical dynamics.

9:00 **IO29:** **Mario Piris** (Donostia International Physics Center, Spain)
Recent Advances in Natural Orbital Functional Theory: Insights into Molecular Dynamics and Beyond.

9:30 **IO30:** **Lichang Wang** (Southern Illinois University, USA)
Molecular Dynamics Simulation-Assisted Electronic Structure Calculations for Studying Electronic Properties of Molecular Systems

10:00 **CO15:** **Xiaoguang G. Zhang** (University of Florida, USA)
First Principles Calculations of Near-Resonance Raman Intensity as Sensitive Tool for Magnetic Molecules

10:25 **F6:** **Rochelle Ferns** (University of St Andrews, United Kingdom)
Stereochemistry of the insertion of diphenylacetylene in a Magnesium(I) dimer.

10:35 ***Coffee break***

SESSION 13 – Chair: Ugo Ancarani

11:00 **IO31:** **Stella Stopkowicz** (Saarland University, Germany)
Spectra from magnetic white dwarf stars and electronic structure in strong magnetic fields.

11:30 **IO32:** **Alessandro Genoni** (Politecnico di Milano, Italy)
X-ray restrained wavefunction approach: a useful tool for density functional theory?

11:55 **CO15:** **Antonio Sarsa** (Universidad de Córdoba, Spain)
Electronic Structure Calculations in Stark Broadening of Balmer Emission Line in Plasmas.

12:15 **CO16:** **Agnieszka Krzemińska** (Łódź University of Technology, Poland)
Multiconfigurational SAPT application to study molecular interactions in $\pi \rightarrow \pi^*$ excited states of anisole complexes.

12:35 **F7:** **Sambit K. Das** (Stockholm University, Sweden)
Transient X-ray absorption signatures resolve the non-adiabatic pathway of Thiopyridone.

12:45 ***Lunch***

SESSION 14 – Chair: David Tew

14:10 **IO33:** **Sonia Coriani** (Technical University of Denmark, Denmark)
Theoretical X-ray spectroscopy to unravel ultrafast relaxation pathways in functional molecules.

14:40 **IO34:** **Seiichiro Ten-no** (Kobe University, Japan)
Explicitly correlated selected coupled-cluster via projective transcorrelation.

15:10 **CO17:** **Raffaele Resta** (CNR-IOM Istituto Officina dei Materiali, Italy)
Berry curvatures and adiabatic phenomena in molecular physics.

15:35 **CO18:** **Edison Salazar** (Instituut-Lorentz, Universiteit Leiden, Netherlands)
Nonadiabatic dynamics using SA-OO-VQE surface hopping: Formaldimine molecule as a case study.

15:55 **F8:** **Davide Materia** (Università degli Studi dell'Aquila, Italy)
Quantum Information Theory for Quantum Chemistry beyond MPS and the advantage of Natural Orbitals.

16:05 ***Coffee break***

SESSION 15 – Chair: Sonia Coriani

16:30 **IO35:** **Barak Hirshberg** (Tel Aviv University, Israel)
Quadratic scaling bosonic path integral molecular dynamics.

17:00 **CO19:** **Kousik Samanta** (Indian Institute of Technology Bhubaneswar, India)
Catching a Glimpse of the Transient States — A Multiconfigurational View.

17:20 **CO20:** **Lars Urban** (University of Munich, Germany)
Efficient Exploitation of Numerical Quadrature in Explicitly Correlated F12 Theory.

17:35 **F9:** **Supriyo Santra** (Indian Association for the Cultivation of Science, India)
Deciphering the mechanism of singlet fission in carotenoids.

17:45 **IO36:** **Jordi Ribas- Ariño** (Universitat de Barcelona, Spain)
Optimal use of oriented external fields to control reactivity.

18:15 **Closing Remarks and MES 2026 Announcement**

20:00 ***Conference dinner***