VII CONGRESSO DELLA DIVISIONE DI CHIMICA TEORICA E COMPUTAZIONALE - DCTC2022

Wednesday, Sep. 21

14:15 - 14:30 **Opening remarks** (**M.C.Menziani** , President DCTC)

Session 1 Chairperson: **C. Adamo**

14:30 - 15:00 **Invited talk: E. Bodo** Computational approaches for biocompatible ionic liquids.

15:00 - 15:15 **M. Gandolfi** Functional groups in chemistry: molecular dynamics experiments.

15:15 - 15.30 **F. Lipparini** CASSCF energy and properties with the Cholesky Decomposition of the two-electron integrals.

15:30 - 15.45 **F. Di Maiolo** Harvesting triplet excitons in TADF emitters with negative singlet-triplet gap: The path towards highly efficient OLEDs.

15:45 - 16:00 **A.N. Nardi** Modelling charge transfer reactions by hopping between electronic ground state minima: application to hole transfer between DNA bases.

16:00 - 16:30 **Coffee break**

Session 2 Chairperson: **G. Mazzone**

16:30 - 17:00 **Invited talk: M. Pagliai** Hydrogen Bond Structure and Dynamics in Liquid Water under Pressure.

17:00 - 17:15 **C.G. Chen** PyMM: An open-source Python program for QM/MM Simulations based on the Perturbed Matrix Method.

17:15 - 17:30 **E. Falbo** Integration of Quantum Chemistry, Statistical Mechanics and Artificial Intelligence for Computational Spectroscopy: the UV-vis spectrum of TEMPO radical in different solvents.

17:30 - 17:45 **A. Pecoraro** Exotic hexagonal structured NaCl films on a methylammonium lead iodide substrate: a first- principles study.

17:45 - 18:00 **D. Fazzi** Polarons in organic conjugated materials: interplay between electronic and vibrational properties.

Thursday, Sep. 22

Session 3 Chairperson: **M. Pavone**

9:00 - 9:30 **Invited talk: G. Raos** Polymers interacting with surfaces: insights and surprises from simple models.
9:30 - 9:45 **M. Bertani** Extending the simulation of NMR parameters of oxide glasses to large models via machine learning.
9:45 - 10.00 **M. Fortino** Theoretical predictions of chiral hybrid perovskites.
10.00 - 10.15 **A. Pierini** Computational modeling of electron-transfer reactivity in aprotic metal-oxygen batteries.
10.15 - 10.30 **M. Monti** A computational approach for modelling Electronic Circular Dichroism of solvated chromophores.

10:30 - 11:00 **Coffee break**

Session 4 Chairperson: **I. Daidone**

11:00 - 11:30 **Invited talk: M. Corno** Cyclodextrin-based nanosponges (CD-NS) as drug delivery systems: a novel computational approach.
11:30 - 11:45 **M. Delle Piane** Reconstructing Reactivity in Dynamic Host-Guest Systems at Atomistic Resolution.
11:45 - 12:00 **A. Pallini** A New Self-Consistent Empirical Potential Model for Multicomponent Borate, Borosilicate and Aluminoborate Glasses.
12:00 - 12:15 **M. Vanzan** Energy transfer to molecular adsorbates by transient hot-electron tunnelling.

12:15 - 14:30 **Lunch and Poster session**

Session 5 Chairperson: **M. Zerbetto**

14:30 - 15:00 **Invited talk: T. Marino** Computational Enzymology: A Challenge for Multiscale Approaches.

15:00 - 15:15 **A. Ciancetta** Predicting G Protein-Coupled Receptor dimers 3D structures in native-like environments.

15:15 - 15:30 **M. Capone** Multi-Scale Modeling of Mechanistic Promiscuity in Glu-ER Mutants Electron-Donor-Acceptor.

15:30 - 15:45 **M. Salha** Manifold Al-Coordination as Nano-Pivots in Porous Cement Nanoclusters.

15:45 - 16:00 **A. Bartocci** Capturing the recognition dynamics of para-sulfonato-calix[4]arenes by cytochrome c: towards a quantitative free energy assessment.

16:00 - 16:30 **Coffee break**

Session 6 Chairperson: **M. Mendolicchio**

16:30 - 16:45 **S. Russo** Modelling amino-acid based ionic liquids with polarizable force field.

16:45 - 17:00 **F. Perrella** Unveiling ultrafast charge transfer in Ruthenium-based metal complexes through ab initio electronic dynamics.

17:00 - 17:15 **F. Ponte** Novel Ru(II)-based compounds active in PDT and PACT cancer therapy: theoretical study of the photophysical properties and photoactivity.

17:15 - 17:30 **A. Massaro** Oxygen redox activity in high-energy Na-ion battery cathodes unveiled from first principles.

17:30 - 17:45 **D. Toffoli** Exploring the surface chemistry of Boroxine- containing frameworks via computational core-electron spectroscopies.

17:45 - 18:30 **DCTC board meeting**

Friday, Sep. 23

Session 7 Chairperson: **C. Greco**

9:00 - 9:30 **Invited talk: S. Corni** Exploring quantum chemistry on quantum computers.

9:30 - 9:45 **S. Di Grande** Novel explicitly correlated composite schemes for the accurate thermochemistry and kinetics of gas- phase reactions.

9:45 - 10:00 **Y. Dai** Solvatochromic Emission from the "Dark" Double- Exciton state of a Polyhalogenated Thiele Hydrocarbon: a quantum-chemical investigation.

10:00 - 10:15 **S. Motta** Investigation of chemokine receptors dimerization through coarse grained metadynamics.

10:15 - 10:45 **Coffee break**

Session 8 Chairperson: **M. Pavone**

10:45 - 11:00 **M. Cioni** Into the dynamics of a metal surface via machine learning of atomic environments.

11:00 - 11:15 **T.D. Marforio** In silico Design of Biocompatible Carborane Carriers for Boron Neutron Capture Therapy.

11:15 - 11:30 **G. Di Liberto** Role of Dihydride and Dihydrogen Complexes in Hydrogen Evolution Reaction.

Session 9 Chairperson: **G. Fronzoni**
Awards, Medals, and final greetings.

11:30 - 11:35 Roetti, Scrocco, Del Re, and Nordio award winners announcement

11:35 - 11:50 Del Re award: **D. Accomasso** *Premio Del Re* Singlet fission dynamics in molecular crystals and covalent dimers.

11:50 - 12:05 Scrocco award: **F. Segatta** *Premio Scrocco* From quantum chemistry to spectroscopy: systems, methods and insight.

12:05 - 12:20 Roetti award: **A.B. Muñoz García** *Premio Roetti* A Quantum-Mechanical Journey Across Renewable Energies: a Tale of Stone, Water and Light.

12:20 - 12:25 materials an Open Access Journal by MDPI **Best Oral Presentation Award**

12:25 - 12:35 **Closing remarks**