Virtual Symposium on Chemical Theory and Computation (VS-CTC)

Monday December 21

2.15 – 3.00 pm: Winners "Miglior Lavoro scientifico"

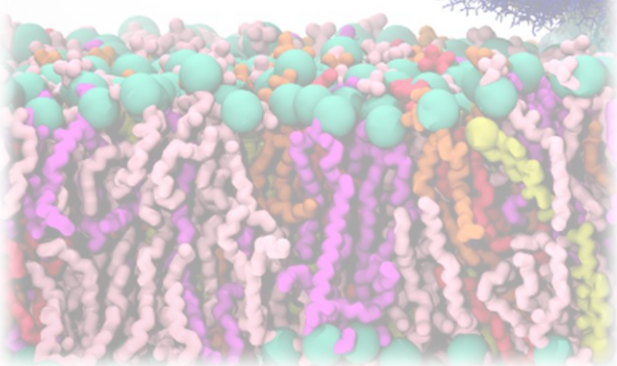
- **Fortuna Ponte** - *Insights from Computations on the Mechanism of Reduction by Ascorbic Acid of Pt^{IV} Prodrugs with Asplatin and Its Chlorido and Bromido Analogues as Model Systems.*
- **Jacopo Fregoni** - *Strong Coupling with Light Enhances the Photoisomerization Quantum Yield of Azobenzene.*
- **Silvia Alessandrini** - *Extension of the "Cheap" Composite Approach to Noncovalent Interactions: The jun-ChS Scheme*.
- **Francesco Di Maiolo** - *Dynamical Disorder and Resonance Energy Transfer: a Novel Quantum-Classical Approach.*

3.00 – 3.50 pm: 1st Flash Talk Session

- **Federica Lodesani** - *Study of lithium disilicate crystallization from melt using well- tempered metadynamics.*
- **Andrea Phan** - *Modelling TADF emitters: a joint theoretical and experimental study.*
- **Francesca Fasulo** - *Ab initio study of singlet Oxygen formation at Li-air battery cathode*.
- **Stefano Pantaleone** - *Schreibersite: a meteor which brings life.*
- **Martina Nucci** - *Mechanochemical improvement of norbornadiene-based molecular solar-thermal systems performance.*
- **Yasi Dai** - *Exploring the low-lying double-exciton state of conjugated diradicals with cost-effective single-reference and multi-reference approaches*.
- **Angela Parise** - *Inhibition of main protease of SARS-CoV-2 by different candidate drugs from a computational point of view.*
- **Giulio Poli** - *Discovery of monoacylglycerol lipase (MAGL) inhibitors based on a pharmacophore-guided virtual screening study*.
- **Alessandra Gilda Ritacca** - *Reactivity of Cu(II)-TSC (thiosemicarbazone) complexes with glutathione in cytosolic environment. Theoretical study and disentanglement of Cu(II)-reduction mechanism.*

3.50 – 4.00 pm: Discussion

4.00 – 4.20 pm: Virtual Coffee Break and **Poster Session**



4.20 – 5.10 pm: 2nd Flash Talk Session

- **Jonathan Campeggio** - *Multiscale modeling of reaction rates: application to archetypal SN_2 nucleophilic substitutions.*
- **Mariagrazia Fortino** - *Hamiltonian excited state Replica Exchange for photoisomerization processes in conjugated polymers.*
- **Tommaso Nottoli** - *CASSCF second-order algorithm with Cholesky Decomposition of the two-electron integrals matrix.*
- **Anna Perfetto** - *Towards new theoretical approaches for the description of excited state properties and reactivity: A Density Based Approach*.
- **Mirko Vanzan** - *On mechanism of hot-electron injection.*
- **Alessandro Rognoni** - *How many water molecules are needed to solvate one?*
- **Sandra Monica Vieira Pinto** - *A computational insight into the relationship between side chains IR lineshapes and local environment in fibril-like structures.*
- **Marco Mendolicchio** - *A unified GVPT2 treatment of abelian and non-abelian symmetries for the energies and intensities of vibrational spectra*.
- **Anna Rovaletti** - *Hydrogen activation by the aerobic MoCu-dependent CO-dehydrogenase*
- **Diego Sorbelli** - *Unravelling the electronic structure of heavy-element-containing molecules with relativistic approaches: the case of gold dihydride.*

5.10 – 5.20 pm: Discussion

5.20 pm: *CTC Video Contest* & Videos Poll

5.40 – 6.10 pm: *Keynote*

- **Rommie E. Amaro** - *Computational Microscopy of SARS-CoV-2*

6.10 pm: *Conclusions & Greetings*