VIII CONGRESSO NAZIONALE DELLA DIVISIONE DI CHIMICA TEORICA E COMPUTAZIONALE

20 Settembre

13:30 - 15:00	Registrazione
15:00 - 15:15	Apertura del Congresso (Presidente DCTC, Autorità)

Sessione 1 - *Chairperson: Vincenzo Barone*

15:15 - 15:45	**P1: Gianfranco Pacchioni (Università di Milano-Bicocca)** *Modeling Single Atoms Catalysts*
15:45 - 16:00	**O1: Lorenzo Briccolani-Bandini (Università di Firenze)** *Concerted vs. Stepwise Proton Transfer reactions in the [2,2'-bipyridyl]-3,3'-diol molecule: a static and dynamic ab-initio investigation*
16:00 - 16:15	**O2: Vincenzo Vigna (Università della Calabria)** *Exploring Machine Learning Techniques for Molecular Property Prediction*
16:15 - 16:30	**O3: Sara del Galdo (Università di Roma 3)** *On the study of thermoresponsive (adsorbent) species at the nanoscale: the case of polyoxazolines*
16:30 - 16:35	**F1: Patrizia Mazzeo (Università di Pisa)** *A Fast Method for Polarizable QM/MM Excited-State Dynamics in Complex Systems*
16:35 - 16:40	**F2: Gabriele Iuzzolino (Scuola Superiore Meridionale)** *Photophysics of a Nucleic Acid-Protein Photo-Crosslinking Model System in Methanol Solution through AIMD simulation.*
16:40 - 16:45	**F3: Alessio Bartocci (Università di Trento)** *A multiscale approach to decipher allosteric cannabinoid binding at the glycine receptor α1*
16:45 - 17:15	*Coffee Break*

Sessione 2 - *Chairperson: Fabrizia Negri*

17:15 - 17:45	**P2: Massimiliano Aschi** *"There's plenty of room at the" border between classical mechanics and quantum chemistry*
17:45 - 18:00	**O4: Andrea Lombardi (Università di Perugia)** *Enhanced molecular networks by invariant shape coordinates*
18:00 - 18:15	**O5: Ilaria Barlocco (Università di Milano-Bicocca)** *Does the Oxygen Evolution Reaction follow the classical OH*, O*, OOH* path on single atom catalysts?*
18:15 - 18:30	**O6: Yasi Dai (Università di Bologna)** *Ambipolar charge transport in organic semiconductors: the role played by diradical character*
18:30 - 18:45	**O7: Guido Raos (Politecnico di Milano)** *Breaking polymer chains, networks and films, with a computer*
18:45 - 19:00	**S1: Sponsor** *E4 Computer Engineering*

21 Settembre

Sessione 3 - *Chairperson: Mirco Zerbetto*

9:00 - 9:30	**P3: Alessio Petrone (Università di Napoli Federico II)** *First principles methods for photo-induced phenomena and non-equilibrium dynamics*
9:30 - 9:45	**O8: Dario Frassi (Università di Pisa)** *Photoisomerization dynamics of spiropyrans*
9:45 - 10:00	**O9: Riccardo Cortivo (Università di Padova)** *A multiscale approach to coupled nuclear and electronic dynamics: quantum-stochastic Liouville equation*
10:00 - 10:15	**O10: Teodoro Pizza (Università di Salerno)** *Charge and Energy Transfer Kinetics in Ternary Organic Solar Cells*
10:15 - 10:30	**O11: Riccardo Conte (Università di Milano)** *Semiclassical vibrational spectroscopy from small molecules to solvated biomolecules*
10:30 - 11:00	*Coffee Break*

Sessione 4 - *Chairperson: Marco Mendolicchio*

11:00 - 11:30	**P4: Silvia Casassa (Università di Torino)** *CRYSTAL: A program for solid state physics and chemistry*
11:30 - 11:45	**O12: Silvia di Grande (Scuola Normale Superiore)** *Accuracy meets Feasibility for Structural and Spectroscopic Investigations: The Study of DNA Basis Tautomers by Novel Parameter-Free Approaches*
11:45 - 12:00	**O13: Giovanni Bistoni (Università di Perugia)** *Combining High Accuracy and Chemical Insight with Local Coupled Cluster Methods*
12:00 - 12:15	**O14: Pierpaolo D'Antoni (Università di Trieste)** *Boosting hybrid kernel TDDFT with STO by Resolution of Identity: implementation and application to a series of ligand protected nanoalloys*
12:15 - 12:30	**O15: Abderrahmane Semmeq (Università dell'Aquila)** *Dye-encapsulated zeolitic imidazolate framework (ZIF-71) for fluorochromic sensing, insights from Molecular Dynamics and TDDFT*
12:30 - 14:30	*Lunch*

Sessione 5 - *Chairperson: Gloria Mazzone*

14:30 - 15:00	**P5: Cristina Puzzarini (Università di Bologna)** *Unveiling exotic chemistry and molecules in the interstellar medium: The role of quantum-chemical calculations*
15:00 - 15:15	**O16: Edoardo Buttarazzi (Scuola Superiore Meridionale)** *The real-time interplay between the ultrafast charge dynamics and nuclear vibrations in dyes for solar cell technologies*
15:15 - 15:30	**O17: Giacomo Salvadori (Università di Pisa)** *Transient Intermediates in a Bacteriophytochrome Photocycle Revealed by Multiscale Simulations*
15:30 - 15:45	**O18: Adriano Pierini (Università di Roma La Sapienza)** *Mechanistic study of redox mediators in Li-O2 batteries*
15:45 - 15:50	**F4: Michele Casoria (Università di Firenze)** *Structural properties of N-glycosylated Protein*
15:50 - 15:55	**F5: Gioacchino Schifino (Università di Catanzaro)** *Chiral self-organization of meso-tetrakis(4-sulfonatophenyl)porphyrin assisted by molecular rotations*

15:55 - 16:00	**F6: Gabriella Di Genova (Università di Perugia)** *Theoretical investigation on S(1D) insertion reactions leading to the formation of S-bearing species in space*
16:00 - 16:30	*Coffee Break*

Sessione 6: Tavola Rotonda - *Chairperson: Claudio Greco*

16:30 - 17:45	**Tavola Rotonda** *Il finanziamento della Ricerca negli anni del PNRR* • *Carlo Adamo* • *Angela Agostiano* • *Maria Chiara Carrozza* • *Gianluigi Consoli* • *Marco Mancini*
17:45 - 18:30	**Assemblea Divisionale**

Sessione 7: Premi e Medaglie - *Chairperson: Isabella Daidone*

18:30 - 18:35	**Proclamazione dei vincitori** *Premio Roetti*
18:35 - 18:50	**A1: Filippo Lipparini (Università di Pisa)** *New Algorithms and Numerical Strategies from Classical Models to Quantum Chemistry*
20:30	***Cena Sociale*** *Ristorante "La Clessidra"*

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Sessione 8 - *Chairperson: Federico Lazzari*

9:00 - 9:30	**P6: Adriana Pietropaolo (Università di Catanzaro)** *Atomistic simulations of chiral polymers and low-dimensional perovskites*
9:30 - 9:45	**O19: Anna Ranaudo (Università di Milano-Bicocca)** *Guiding competitive binding assays using protein-protein interaction prediction: the affitin-Her2 use case*
9:45 - 10:00	**O20: Annalisa Pallini (Università di Modena-Reggio Emilia)** *Aluminosilicate Glasses: Thermal and Mechanical Properties Simulations*
10:00 - 10:05	**F7: Luigi Crisci (Scuola Normale Superiore)** *Toward a black-box computation of accurate rate constants for barrier-less processes: new hints for a challenging problem*
10:05 - 10:10	**F8: Sergio Rampino (Università di Padova)** *The roto-conformational diffusion tensor as a tool to interpret molecular flexibility*
10:10 - 10:15	**F9: Francesco Ferdinando Summa (Università di Salerno)** *Electronic Current Densities and Origin-Independent Property Densities Induced by Optical Fields*
10:15 - 10:45	*Coffee Break*

Sessione 9 - *Chairperson: Enrico Bodo*

10:45 - 11:00	**O21: Pierraffaele Barretta (Università della Calabria)** *An activatable photosentizer for Photodynamic Therapy: mechanism of NO photo-release and free radical generation*
11:00 - 11:15	**O22: Giulio Poli (Università di Pisa)** *An in silico platform for evaluating the potential pathogenic impact of hRPE65 missense mutations*
11:15 - 11:30	**O23: Roberto Paciotti (Università di Chieti-Pescara)** *The FMO-GRID based scoring functions to predict the binding energy of ligand-receptor complexes containing metals.*

P: Plenary O: Oral F: Flash S: Sponsor A: Award

Sessione 10: Premi e Medaglie - *Chairperson: Giovanna Fronzoni*

11:30 - 11:35	**Proclamazione dei vincitori** *Premi Miglior presentazione (E4 Computer Engineering), Nordio, Del Re, Scrocco*
11:35 - 11:50	**A2: Silvia Alessandrini (Università di Bologna)** *Modelling weak interactions in the gas phase: from non-covalent bond to reactions rates*
11:50 - 12:05	**A3: Matteo Capone (Università dell'Aquila)** *Illuminating PhotosystemII Catalysis: Molecular Insights from QM/MM Simulations*
12:05 - 12:15	*Saluti*