Poster Session

Phase Stability Simulation of Copper Chalkogenide Nanoparticles From First Principles
Beqiraj Alkit
Institut für Chemie, Universität Potsdam, Postdam, Germany

Spectroscopic properties of polymetallic chains with direct metal-metal bonds: DFT and CASSCF studies
Mohammed Obies AL-Nafee
Physical and Theoretical Chemistry Laboratory, University of Oxford, Oxford, UK

Non-Fluorescent J-Aggregates of Quadrupolar Chromophores: A Theoretical Description Beyond the Exciton Picture
Brunella Bardi
Dipartimento di Scienze Chimiche, della Vita e della Sostenibilità Ambientale, Università di Parma, Parma, Italy

H_2 dissociation and H_2O evolution over pristine and silver decorated CeO_2(111): a computational study
Luca Brugnoli
Dipartimento di Scienze Chimiche e Geologiche, Università di Modena e Reggio-Emilia, Modena, Italy

Study of the tautomerism reaction through a pump-probe experiment
Bastien Casier
Sorbonne Université, CNRS, Laboratoire de Chimie-Physique, Matière et Rayonnement, Paris, France

First Steps towards Unravelling the Working Mechanisms of a BODIPY-based Molecular Rotor for Sensing Viscosity
Bethan Cornell
Kings College London, Physics Department Strand, London, UK

Composition of Earth's Core: A Proposal Based on First-principles Study of Phonon and Elastic Properties of Fe-C and Fe-Ni Solids
Tilak Das
Department of Physical Sciences, Indian Institute of Science Education and Research, Kolkata, Mohanpur Campus, Nadia, West Bengal, India

First-principles insight into heterogeneous photocatalysis at a photoactive Ru-complex on a covalent Triazine framework
Arthur De Vos
Center for Molecular Modeling, Ghent University, Zwijnaarde, Belgium

Computational study of the electronic structure and magnetic properties of organic diradicals and their complexes with 3d-metal cations
Dmitry E. Gorbunov
Department of Physics, Novosibirsk State University, Novosibirsk, Russia
Institute of Chemical Kinetics and Combustion of SB RAS, Novosibirsk, Russia

Partial charge profiles of fluorophores: modelling the effect of solvent and excitation
Duncan Gowland
Department of Physics, King's College London, London, UK

Understanding phase transformations in flexible metal-organic frameworks using computational vibrational spectroscopy
Alexander E.J. Hoffman
Center for Molecular Modeling, Ghent University, Zwijnaarde, Belgium

A Hybrid QM/MM Study of the Fluorescence Mechanism of Infrared Fluorescent Proteins
Tristan Mackenzie
Department of Chemistry, Imperial College London, London, UK

Fluorescence enhancement via electronic reprogramming of a sensory microbial rhodopsin
María del Carmen Marín Pérez
Biotechnology, Pharmacy and Chemistry Department, University of Siena, Siena, Italy.

Benchmarking Double-Hybrid Density Functionals on excited electronic states
Carmela Morgillo
Chimie ParisTech, PSL Research University, CNRS, Institut de Recherche de Chimie Paris 11, Paris, France

Rational design of Near-Infrared absorbing D-π-A organic dye molecules
Ayush K. Narsaria
Department of Theoretical Chemistry, Vrije Universiteit Amsterdam, Amsterdam, The Netherlands

Tuned Quantification of Particle-Hole Distance in Charge-Transfer Excitations: a Revised Version of the DCT Index
Anna Perfetto

Chimie ParisTech, PSL Research University, CNRS, Institut de Recherche de Chimie Paris, Paris, France

Wavefunction Frozen Density Embedding: an analysis of the errors in excitation energies
Niccolò Ricardi
Department of Physical Chemistry, University of Geneva, Geneva, Switzerland

From Single Molecule to Full Monolayer Adsorption of Dopamine on TiO_2 surface
Costanza Ronchi
Dipartimento di Scienza dei Materiali, Università di Milano-Bicocca, Milano, Italy

Ab initio study of copper oxides as an alternative to nickel oxide in photocathodes for dye-sensitized solar cells
Eduardo Schiavo
Department of Chemical Sciences, University of Naples "Federico II"; Napoli, Italy

1-Dimensional inorganic double helices as information storage materials
Maximilian A. Springer
Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Fakultät für Chemie und Mineralogie, Universität Leipzig, Leipzig, Germany

PyDEF: an easy to use post-treatment software for ab-initio calculations
Adrien Stoliaroff
Institut des Matériaux Jean Rouxel (IMN), Université de Nantes, CNRS, Nantes Cedex 3, France

Predicting Linear Absorption in Dissipative Macromolecular Systems
Michele Turelli
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