Journées Théorie, Modélisation et Simulations - JTMS 2020

Monday, 2nd of November

Session 1: Methods (excited states and correlated systems)

13h50 Introduction

14h00 Pierre-François Loos (conférence invitée)
Higher roots of the Schrödinger equation

14h40 David Grégoire
SCF methods for excited states in strong magnetic fields

15h00 Saad Yalouz
A state-averaged quantum algorithm for an equal footing description of ground and excited states on a near term quantum computer

15h20 Sajanthan Sekaran
Quantum embedding for strongly correlated systems

15h40 Mauricio Antonio Rodríguez Mayorga
Improved density matrices from GW approximation

16h00 Posters flash: *Mohammad Asad, Christian Brouder, Miguel Escobar Azor, Guillaume Bareigts, Johanna Klein, Richard Asamoah Opoku, Agota Toth, Xiang Yuan, Gaétan Laurens, Mehdi Benmameri*

Tuesday, 3rd of November

Session 2: Spectroscopies and interfaces

10h00 Guillaume Le Breton
Second Harmonic Generation at liquid interface: a multi-scale numerical approach

10h20 Juliette Lainé
Molecular understanding of adsorption mechanisms of fatty acids on fluorite under flotation conditions

10h40 Anagha Sasikumar
Relative importance of ring currents and adsorption energies in the determination of in situ NMR spectra

11h00 Roxanne Berthin
The water behavior at electrochemical interfaces: a synergy among molecular dynamics, electrochemistry and Nuclear Magnetic Resonance spectroscopy

11h20 Nawras Abidi
Revisiting the active sites on MoS2 in aqueous solution via grand-canonical DFT: The role of water dissociation

11h40 Paul Clabaut
Investigating solvation at metal/water interfaces: the SolvHybrid tool fueled by the GAL forcefield

Session 3: Methods (machine learning and various)

14h00 Julien Lam
Gold-Iron interactions in nanoparticles modeled by physically motivated machine learning potential

14h20 Isaac Chantrenne
Discovery of new thermoelectric octahedral transition-metal cluster chalcogenides assisted by artificial intelligence

14h40 Guillaume Hoffmann
Predicting experimental electrophilicities with quantum descriptors : from standard to non linear approaches

15h00 Miquel Huix-Rotllant
Linear scaling electrostatic embedding QM/MM based on electrostatic potential fitted atomic charges

15h20 Laura Scalfi
A semi-classical Thomas-Fermi model to tune the metallicity of electrodes in molecular simulations

15h40 Pascal Pernot
You should not use the mean absolute error to choose a Quantum Chemistry method

16h00 Posters flash: *Mohamed Bensifia, Aimeric Dabin, Théophile Gaudin, Tom Irons, David Lacoste, Roland Panzou, Weiliang Ma, Heng Zhang, Amit Sahu*

Wednesday, 4th of November

Session 4: Biology (and molecules of biological interest)

10h00 Xiaojing Wu (prix Gaston Berthier)
Simulation of heme proteins with polarizable force field

10h40 Olivier Languin-Cattoën
How do protein conformations define the catch-bond behavior of a bacterial pili?

11h00 Abderrahmane Semmeq
DNA under ionizing radiation: The peculiar effect of water

11h20 Ayoub Daouli
Tuning the properties of faujasite nanozeolites for optimal capture of O_2/CO_2

11h40 Mariia Savenko
Assessing structure and stability of supported lipid bilayers on graphene oxides and silica using all atom molecular dynamics simulations

Session 5: Simulations for a variety of applications

14h00 Arthur Hagopian
Thermodynamic origin of dendrite growth in metal anode batteries

14h20 Erika Fallacara
Order and disorder in KOH and KOD crystals

14h40 Rabii Larhlimi
Up to eight nitrogen per bismuth in high pressure BiN_x phases (x =1-3, 6, 8)

15h00 Dominika Lesnicki
Field-dependent ionic conductivities from molecular dynamics simulations

15h20 Thomas Mangin
Eu^{3+} extraction to ionic liquids by BTP ligands: Interface crossing studied by MD and PMF simulations

15h40 Vincent Delmas
On the reliability of acquiring molecular junction parameters by Lorentzian fitting of I/V curves

Thursday, 5th of November

Session 6: Spectroscopies (no interfaces)

10h00 Aurélie Falcone
Raman spectroscopy for energy materials

10h20 Aseem Rajan Kshirsagar
Optical properties of photoresponsive MOFs: assessing fragment models using the BSE/GW formalism

10h40 Hanna Oher
A combined ab initio and time-resolved laser-induced fluorescence study of uranium-ligand interactions

11h00 Manon Bousquet
Understanding the optical signatures of exotic benzoquinonemonoimine (BQI) π-zwitterions

11h20 Laurie Lescos
Performance of DFT functionals for calculating second-order nonlinear optical properties of merocyanine dyes

11h40 Juan Sanz Garcia
Unraveling the luminescent pathways of the NanoLuc-furimamide complex

Session 7: Reactivity

14h00 Antoine Geoffroy
Theoretical study of Diels-Alder Reaction's asynchronicity with DFT and topological descriptors

14h20 Radhika Gupta
Theoretical assessment of "fuzzy" chemical concepts: from chemical bond descriptors to reactivity

14h40 Gabriel Breuil
Photo-isomerization of oligo(phenyl-acetylenes) in their first electronic excited states

15h00 Elise Lognon
Dihydropyrene photoisomerization mechanism revisited with spin-flip time-dependent density functional theory.

15h20 Lucien Dupuy
Quantum cumulative reaction probability in deep tunneling regime from classical-like trajectory simulations

15h40 Yaidel Toledo-Gonzalez
Molecular design for catalytic activities of helical chiral oligoureas

Friday, 6th of November

Session 8: Biology (transport, origin of life)

10h00 Nathalie Basdevant (conférence invitée)
Coarse-grained modelling of transport through protein nanopores

10h40 Angelika Janaszkiewicz
Modeling protein-mediated transport in kidney cells: in silico pharmacology of Organic Anion Transporters

11h00 Mario Rocha
Molecular Dynamics simulations of a DNA-based biosensor: How a conformational switch deciphers and predicts the transduction process

11h20 Vishal Kumar Porwal
Microscopic understanding of the nanoconfined environment within hybrid layered double hydroxides

11h40 Alejandro Diaz Marquez
Molecular basis for thermophoresis in aqueous solutions

12h00 Concluding remarks