Journées Théorie, Modélisation et Simulations - JTMS 2022

Amphi Daniel Grandjean, Bâtiment 10B, Institut des Sciences Chimiques de Rennes

Thursday 13th of October

09:30	**Welcome**	
09:40	New interpretation of the reduced density matrices	Thierry Deutsch
10:20	Reference energies for cyclobutadiene: automerization and excited states	Enzo Monino
10:40	Non-adiabatic coupling in trajectory surface hopping: How approximations impact excited-state reaction dynamics	Isabella Meritt
11:00	Poly-epoxy amine polymer surfaces: Simulation of XPS spectra and insights in their metallization mechanism	Fatah Chiter
11:20	Computational characterization of the non-linear optical properties in solution and preliminary analysis in clusters of molecular photoswitches	Angela Dellai
11:40	Understanding the conformational flexibility of large aromatic ligands of organolanthanides	Valeriu Cemortan
12:00	**Lunch**	
13:00	**Poster session**	
14:20	Atomic scale simulation of intricate aluminosilicate catalysts: structural and mechanical sources of complexity	Céline Chizallet
15:00	Isomerization and cracking of alkenes catalyzed by zeolites: from *ab initio* molecular dynamics to machine learning perturbation	Jérôme Rey
15:20	Why silver zeolites are efficient for radioiodine capture? A mechanistic description by a*b initio* molecular dynamics	Michael Badawi
15:40	Critical comparison of molecular dynamics simulations of amorphous Metal-Organic frameworks	Nicolas Castel
16:00	Trapping properties of iodine in actinide oxides: A DFT+U study	Mathieu Gascoin
16:20	**Coffee break**	
16:40	Computation of vibrational circular dichroism in the periodic gauge	Sascha Jähnigen
17:00	A selected configuration interaction study of ground- and excited-state dipole moments and oscillator strengths	Yann Damour
17:20	Theoretical study of the vibrational energy redistribution in CO and CO:N_2 aggregates	Samuel Del Fré
17:40	Ultrafast calculation of solvation in supercritical CO_2 with classical DFT	Antoine Carof

Friday 14th of October

09:00	Simulating the birth of a cellular organelle: molecular mechanism of lipid droplet budding	Luca Monticelli
09:40	*In vivo* stability of ^{211}At radiopharmaceuticals : on the impact of halogen bond formation	Thibault Yssartier
10:00	Molecular simulations of CH_4 adsorption in kerogen: Effects of maturity and poromechanics	Kévin Potier
10:20	Molecular dynamics investigation of non-Fickian effects on desorption from source rocks' organic matter	Amaël Obliger
10:40	**Coffee break**	
11:00	A density-based basis set correction for wave-function methods: Overview of recent developments ad results	Emmanuel Giner
11:20	Coupling of quantum chemical models and high performance algorithms for the global exploration of the energy landscape of atomic and molecular systems	Valentin Milia
11:40	BSE-GW excited-state surfaces: tackling the DMABN twist challenge	Iryna Knysh
12:00	Reducing computational cost of geminal methods for strongly-correlated electrons	Patrick Cassam-Chenai
12:20	Artifical neural networks as exchange and correlations functionals for transition metal complexes	Joao Paulo Almeida de Mendonca
12:40	**Lunch**	
14:00	Halide perovskites beyond methylammonium lead iodide	Mikaël Kepenekian
14:40	Photochrom grafted gold nanoparticle for solar energy harvest and storage	Corentin Poidevin
15:00	Impact of the electric field on magnetic parameters: Disruptive Dzyaloshinskii-Moriya interaction	Barthélémy Pradines
15:20	Unravelling the spin-phonon relaxation mechanism in a series of Co(II) and Dy(III) single-molecule magnets	Sourav Mondal
15:40	Rigorous extraction of magnetic exchange couplings in compounds with several magnetic centres: The recomposition method	Grégoire David
16:00	**End of JTMS**	

Posters

13:00-14:20 (13th of October)

P1	Hylight, a new open-source tool for the luminescence simulation of inorganic materials	Théo Cavignac
P2	*Ab initio* simulations of the hydration of organic compounds relevant to atmospheric aerosols	Rodolphe Pollet
P3	Frequency dependent conductivity and electrical current fluctuations of confined electrolytes	Minh-Thê Hoang Ngoc
P4	DFT screening of monovalent and divalent cation embedded faujasite on the selective entrapment of NO and NO_2 in the presence of H_2O	Ioannis Karamanis
P5	Intepretation of NMR spectra of aqueous systems in porous carbons using lattice simulations	Céline Merlet
P6	Chemistry and thermodynamic properties of proactinium (V) in aqueous phase by *ab initio* calculation	Hanna Oher
P7	Why ultrafast photoinduced CO desorption dominates over oxidation on Ru(0001)	Auguste Tetenoire
P8	*Ab initio* screening of divalent cations embedded in chabazite for separation operations involving CH_4, CO_2, H_2 and N_2	Jérôme Rey
P9	Modelling absorption spectra of furimamide - nanoluciferase system	Houda Moumene
P10	Molecular dynamics simulations unravelling the influence of light-activated drugs on a membrane cell model	Anastasiia Delova
P11	2D proton diffusion in model potentials and assessment of quantum MD methods	Niccolò Avallone
P12	Prediction of Lewis acidity of borane derivatives with constrained ligands via Machine Learning	Juliette Fenogli
P13	Modelling bound and unbound RNA structures using molecular dynamics simulations to unravel the relationship between structure, flexibility and chemical reactivity	Elisa Frezza
P14	Toward a molecular picture of thermal denaturation of RNA duplexes	Aimeric Dabin
P15	DFT quantum chemical studies of luminescent copper (I) compounds	Raquel Utrera Melero
P16	Quantum chemistry of chromophores for OLED applications	Maxime Hodée

P17	Ab initio investigation of the mechanical and electronic properties of bismuth vanadate $BiVO_4$	David Vincent
P18	Crucial role of conjugation in monolayer-protected metal clusters with aromatic ligands	Hans-Christian Weissker
P19	$(PdHCu_{11}\{S_2P(OiPr)_2\}_6(C{\equiv}CPh)_4)$ a hybride-containing 2-electron superatom as electrocatayst for hydrogen production	Hao Liang
P20	Electronic structures and bonding properties of organometallic palladium nanoclusters	Jianyu Wei
P21	Study of the bending relaxation of water by collision with Ar using the Rigid Bender Close Coupling treatment	Ricardo Manuel Garcia Vázquez
P22	Organolanthanide complexes: ab initio study of electronic structures and rationalization of magnetic properties	Léo La Droitte