Journées Théorie, Modélisation et Simulations - JTMS 2023

Société Chimique de France

Société Française de Physique

ThéMoSiA
Théories - Modélisations - Simulations - Atomistiques

Tuesday 17th of October

	09:30	**Welcome**	
Chair: Claire Lemarchand	**09:40**	Nanoparticles growth mechanisms, morphology and electronic properties	Magali Benoit
	10:20	Mesoscopic simulations of coatings using the electrophoretic process in aqueous suspensions	Mélina Noblesse
	10:40	Molecular simulations study of the adsorption dynamics of ions on carbon electrodes	Nicolas Gaudy
	11:00	Dynamics of hydrogen adsorption and dissociation on nitrogen covered tungsten surface	Ohmar Norhan
	11:20	Theory of spin crossover molecules on metal surfaces: The effect of ligand doping	Rémi Pasquier
	11:40	A system-bath model to investigate the interaction of a molecule with its environment	Loïse Attal
	12:00	**Lunch**	
	13:00	**Poster session**	
Chair: Benjamin Lasorne	**14:00**	Theories and simulations of ultrafast processes in molecules	Federica Agostini
	14:40	Non-adiabatic dynamics with trajectory surface hopping: Benchmarking electronic structure methods on azomethane photoisomerization	Thomas Papineau
	15:00	Dissociation and isomerization upon ionisation of ethylene: A non-adiabatic dynamics perspective	Lina Fransen
	15:20	An exact factorization perspective on dynamics around conical intersections: On the nature of topological and geometric phases in molecules	Lea Ibele
	15:40	Quantum dynamics around PPE's conical intersections for spectroscopic and real-time studies	Galiana Joachim
	16:00	Deciphering the secrets of madder molecules through computational chemistry	Linh Tran
	16:20	**Coffee break**	
Chair: Pascal Larregaray	**16:40**	Simulation of the equilibrium and the transport of ions at the liquid-liquid interface	Lara Ziberna
	17:00	Molecular prediction of lanthanide cation transfer for liquid-liquid extraction	Erwann Guillam
	17:20	Aggregation phenomenon and effects of trapped compounds in complex mixture by molecular dynamics simulations	Luis Acevedo Fernandez
	17:40	Mechanism of excess proton transport in water revealed by neural network-based path integral molecular dynamics simulations	Axel Gomez

Wednesday 18th of October

Chair: Marc Baaden	**09:00**	Exploring protein-protein interaction networks in 3D under the lens of coevolution	Raphaël Guérois
	09:40	Agnostic exploration of a new pathway for prebiotic glycine synthesis by ab initio and machine learning molecular dynamic	Léon Huet
	10:00	Free-energy landscapes of an intrinsically disordered protein: Alpha-synuclein	Patrick Senet
	10:20	A new neural network interatomic potential for the simulation of the thermal and mechanical properties of silica zeolites	Luca Brognoli
	10:40	**Coffee break**	
Chair: Rémi Maurice	**11:00**	Study of photophysical properties of azaBODIPY compounds through vibronic calculations	Ludmilla Verrieux
	11:20	Spin–vibronic mechanism at work in a luminescent square-planar cyclometalated tridentate Pt(II) complex: Absorption and ultrafast photophysics	Mandal Souvik
	11:40	Joint experimental and theoretical investigation of excited state vibrational coherences in Mn single molecule magnets	Julien Eng
	12:00	Modifications of Tanabe-Sugano d6 diagram induced by radical ligand field: Ab initio inspection of a Fe(II)-verdazyl molecular complex	Pablo Roseiro
	12:20	Reference energies for valence ionizations and satellite transitions	Antoine Marie
	12:40	**Lunch + Posters**	
Chair: Bruno Senjean	**14:00**	The QuantNBody package: A numerical platform for methodology development in quantum chemistry	Saad Yalouz
	14:40	Divide and conquer embedding approach for electronic structure calculation	Quentin Marecat
	15:00	A new variational density matrix formalism for correlated systems	Matthieu Vladaj
	15:20	One dimensional model for relativistic quantum chemistry	Timothée Audet
	15:40	DFTB molecular dynamics for a quantitatively accurate description of the experimental absorption bands of solvated organic switches.	Benjamin Ludwig
	16:00	**End of JTMS**	

Posters

13:00-14:00 (17th of October)

P1	Molecular insight into the photonastic phenomenon: Study of the coupling between the photochemical reaction and the intramolecular relaxation of the polymer	Marta Serrano Martínez
P2	Computational Analysis of Structural Changes in Photoswitchable Systems using Molecular Simulations	Orlando Villegas
P3	Effect of inorganic ligands on Pa5+ and PaO3+ relative stabilities: A computational study	Tamara Shaaban
P4	Computing RedOx properties in solution	Maxime Labat
P5	Some thoughts on the quantum mechanical definition of the mean square displacement	Roberto Marquardt
P6	Computation of exchange couplings in photogenerated excited states in DFT-KS	Grégoire David
P7	Optimized excitonic transport mediated by local energy defects: Survival of optimization laws in the presence of dephasing	Lucie Pepe
P8	How the pH of aqueous droplets and its size dependence are controlled by the air-water interface acidity	Miguel de la Puente
P9	Quantum embedding strategy for describing multiple electronic states	Filip Cernatic
P10	Exploring surface terminations and reactivity in epitaxially grown maghemite on Pt substrates through first principles	Amit Sahu
P11	State-specific coupled-cluster methods for excited states	Yann Damour
P12	Recent developments in molecular excited-state dynamics with the exact factorization	Eduarda Sangiogo Gil
P13	A comparison of the shock properties of three polymer melts: A molecular dynamics study	Claire Lemarchand
P14	Spectroscopic properties in vibrational strong coupling in disordered matter from Path - Integral simulations	Jaime De la Fuente Diez
P15	Physical properties of 2D multilayered perovskites and 2D/3D bilayers	Claudine Katan
P16	Investigation of a germanium induced √109 x √109 reconstruction on Ag(111): Germanene or not germanene ?	Marie-Christine Hanf

P17	Exact excited-state functionals of the asymmetric hubbard dimer	Sara Giarrusso
P18	DFT calculation for heteroleptic silver-rich 8-electron superatoms	Hao Liang
P19	^{25}Mg and ^{67}Zn NMR study of $Mg_xZn_{1-x}O$ solid solutions: Observing correlated disorder	Aël Cador
P20	Immobilization effect on optical properties of quantum dots transferred from solution to surfaces probed by nonlinear optical spectroscopy	Emeline Boyer
P21	Dynamics of hydrogen interaction on tungsten surfaces	Laura Viaud
P22	Supramolecular auto-assembly of small peptides. Studies by molecular dynamics	Tetiana Dorosh
P23	UV-spectrum and photo-decomposition of peroxynitrous acid in the troposphere	Wiem Chebbi
P24	ESIPT-capable zinc(II) complexes with 1-hydroxy-1H-imidazole-based ligands: Molecular design and anomalous anti-Kasha emission	Nikita A. Shekhovtsov
P25	Understanding the many-body electronic structure of the nitrogen-vacancy center in diamond	Alan Custodio dos Reis Souza
P26	Modeling of bimetallic nanoparticles synthesized through radiolysis with theoretical chemistry and automated learning	Raphaël Vangheluwe
P27	Energy redistribution upon hydrogen atom scattering of hydrogen-covered W(100) surfaces	Raidel Martin Barrios
P28	Red-emitting tetraphenylethylene derivative with aggregation-induced enhanced emission for luminescent solar concentrators: A combined experimental and density functional theory study	Qinfang Wang
P29	Deciphering the secrets of madder molecules through computational chemistry	Linh Tran