Journées Théorie, Modélisation et Simulations - JTMS 2021

En visioconférence : lien zoom

Thursday 9th of December

09:30	**Welcome**	
09:40	Modeling photonastic materials: insights from the molecular scale	Aurélie Perrier
10:20	Optical properties of photo-switching metal-organic frameworks	Roberta Poloni
10:40	Theoretical chemistry to fight COVID-19: Original MD and QM/MM strategies to validate G-quadruplex folding of SARS-CoV-2 RG-1 RNA	Tom Miclot
11:00	Determination of Vibrational Circular Dichroism spectra of fluxional molecules through classical polarisable molecular dynamics	Jessica Bowles
11:20	Hydrophobicity/hydrophilicity of SAMs/water interfaces investigated by DFT-MD Simulations: A general platform of investigation and a new descriptor	Wanlin Chen
11:40	**Flash presentations**	
12:00	**Lunch**	
13:00	**Poster session**	
14:20	Pulse shape and molecular orientation determine the attosecond charge migration in Caffeine	Thomas Niehaus
15:00	Predicting electron attachment energies using Multi-basis-set TDDFT methods	Guillaume Thiam
15:20	Revisiting the derivative discontinuity problem in ensemble density-functional theory for neutral excitations: an N-centered perspective	Filip Cernatic
15:40	Theoretical study of collisional quenching: Non-adiabatic scattering pathway and on-the-fly surface hopping	Clément Soulié
16:00	Collisional excitation of CO2 by He : New potential energy surface and scattering calculations	Amélie Godard
16:20	**Coffee break**	
16:40	Translational Inelasticity of Hydrogen Atoms Scattering off Hydrogen-Covered W(110) Surfaces	Raidel Martin Barrios
17:00	Origin of Confined Water's Dielectric Constant Reduction	Jean-François Olivieri
17:20	Implementing explicit ion polarisation in electrochemical simulations.	Camille Bacon
17:40	Wettability of clay surfaces and its implication on the status of water in unsaturated porous media	Loïc Guérin

Vendredi 10 décembre

09:00	"Human learning" tools for molecular simulations	Jérôme Hénin
09:40	De novo generation of organic molecular materials	Thomas Cauchy
10:00	Description of Chemical Reactivity using Quantum Chemical Topology	Johanna Klein
10:20	Transitions between alumina (meta)stable phases	Mohammad Hellani
10:40	**Coffee break**	
11:00	Modeling diffusion coefficients of dissolved carbon dioxide in Champagne wines by molecular dynamics simulations	Mohammed Ahmed Khaireh
11:20	Escaping the grain : Atomic-scale simulation of fission gas release in UO2 nuclear fuel	Théo Beigbeder
11:40	Stability and structure of adaptive molecular self-organized aggregates designed for new artificial water channels.	Arthur Hardiagon
12:00	The role of interactions in ionic current fluctuations and conductivity in nanopores, insights from Brownian dynamics and the stochastic Poisson-Nernst-Planck model	Minh-Thê Hoang Ngoc
12:20	Spontaneous propulsion of an isotropic colloid in a phase-separating environment	Jeanne Decayeux
12:40	**Lunch**	
14:00	How to create giant Dzyaloshinskii-Moriya interaction?	Nathalie Guihéry
14:40	DFT study of the reactivity of molybdenum cluster units at the ground and excited state	Nina Tyminska
15:00	Analytical nonadiabatic couplings and gradients on quantum computers: towards excited-state quantum dynamics	Bruno Senjean
15:20	Modeling excited states properties in solid state materials	Camille Latouche
15:40	Computing low energy excitations in strongly correlated systems: RelaxSE	Marie-Bernadette Lepetit
16:00	Ab initio simulations of the hydration of organic compounds relevant to atmospheric aerosols	Rodolphe Pollet
16:20	**End of JTMS**	

Séance posters :

P1	Ab initio simulation of borosilicate glass–water interface	Rodolphe Pollet
P2	Ab initio study of Hydrogen embrittlement in binary nickel alloys	Aman Prasad
P3	Approche théorique de la dimérisation de la chlorophylle (A) dans les mélanges solvant organique – eau : calculs quantochimiques au niveau SMD-DFT-D3	Claude Millot
P4	Bridging NMR experiments and molecular simulations for ions adsorbed in porous carbons	Céline Merlet
P5	Calculation of Rényi entropy in realistic quantum systems	Miha Srdinsek
P6	Core-Level X-Ray Spectroscopies With Relativistic Hamiltonians:The Uranyl Ion Case	Wilken Aldair Misael
P7	From theoretical physics in atomic collisions to applications in nuclear medicine via TILDA-V	Alexandre Larouze
P8	In silico methodology to study regioselectivity modulations of a glycosidase: molecular docking and dynamics approach	Olivier Tasseau
P9	Investigating the interaction of enzymes with functionalized surfaces : Lessons from multiscale modeling approaches	Sophie Sacquin-Mora
P10	Mixed theoretical and experimental approach to better understand and exploit a chemical reaction	Agathe Fayet
P11	Modélisation de systèmes bioluminescents issus des crevettes pour de meilleurs biocapteurs	Houda Moumene
P12	Simulation of radiolysis in organic phases with plutonium	Damien Tolu
P13	Study of acid dissociation at the air-water interface with neural network potentials	Miguel De La Puente
P14	Study of the influence of (de)protonation on photophysical properties for White OLEDs Chromophores	Maxime Hodée
P15	Ab initio study of organolanthanide Single Molecule Magnets	Léo La Droitte
P16	The Monohydration of oxygenated mercury-containing compounds of Atmospheric Interest	Sonia Taamalli
P17	Theoretical studies of chiroptical properties for lanthanide complexes	Maxime Grasser
P18	The moving crude adiabatic alternative to the adiabatic representation in excited state dynamics	Rosa Maskri

P19	Atmospheric gas phase OH-initiated degradation of metazachlor herbicide	Zainab Srour
P20	MoS_2 for unconventional computing and biosensing applications: A first principles study	Gabriele Boschetto
P21	Surface state of heterogenous Ru catalysts in liquid water under gas phase environments	Akif Ramzan Muhammad
P22	A molecular perspective on induced charges on a metallic surface	Giovanni Pireddu
P23	A new approach to interpret copper L-shell photoelectron spectra	Mohammadreza Mosaferi
P24	Second-order nonlinear optical properties of azobenzene switches with bulky substituents	Carmelo Naim
P25	Toward the computation of fluorescence yields	Manon Bousquet
P26	Towards a new class of heterometallic complexes – A theoretical point of view	Valeriu Cemortan
P27	Development of a new parameter set for ReaxFF force field including chloride bonds	Matthieu Wolf
P28	Unravelling the luminescence phenomena in KCl:S : Theory meets experiment	Théo Cavignac
P29	Theoretical study of the magnetic properties of BaNiF4	Julien Lévêque
P30	Development of a reliable protocol to calculate collision cross sections (CCS) of polyphosphodiester polymers	Fiona Fondjo