Journées Théorie, Modélisation et Simulations - JTMS 2024

Tuesday 8th of October

	09:30	**Welcome**	
Chair: Amaël Obliger	**09:40**	Conceptual theoretical methods to address the challenge of energy density in Li-ion batteries	Marie-Liesse Doublet
	10:20	Investigating the effect of particle size and polydispersity on NMR spectra of ions diffusing in disorder porous carbons through a mesoscopic model	El Hassane Lahrar
	10:40	Multi-scale modeling of the dissolution/growth dynamics of metallic copper clusters during synthesis or catalysis processes	Marina Descoubes
	11:00	Studying the phase behavior of clay sheets using a flexible coarse-grained model	Félicien Pauly
	11:20	Colloid aggregation simulations at high particle density using fast lubrication dynamics	Rémi Martin
	11:40	Adapting chemical reaction kinetics of biomass fast pyrolysis to fluidized-bed reactor model	Zoé Mercier
	12:00	**Lunch**	
	13:00	**Poster session**	
Chair: Rémi Maurice	**13:40**	Hydrogen atom scattering from clean and H-covered tungsten surfaces: Recent developments	Pascal Larregaray
	14:20	Non-adiabatic dynamics investigation of $Cr(CO)_4$bpy photodissociation	Bartosz Ciborowski
	14:40	Two-photon vibrational resolved spectra of organic dyes: Insights into the role of Herzberg-Teller couplings	Carmelo Naim
	15:00	Modeling multiple photoinduced electron transfers in covalent donor-photosensitizer-acceptor triads	Nicolas Issot
	15:20	Neural network-based sum-frequency generation spectra of pure and acidified water interfaces with air	Miguel De la Puente
	15:40	Dynamics of hydrogen interaction on tungsten surfaces: quantum or classical?	Laura Viaud
	16:00	**Coffee break**	
Chair: Boris Le Guennic	**16:20**	Point defects and diffusion mechanisms in titanium nitrides (TiN and Ti_2N) including oxygen insertion	Kevin Gautier
	16:40	Computation of exchange couplings in photogenerated excited states in DFT-KS	Grégoire David
	17:00	Ni surfaces and nanoparticles functionalized with trimethylphosphine: A DFT study of structure sensibility, magnetization and topological analysis	Sebastian Godoy
	17:20	Prediction of very large skyrmion stability in monolayer MnSeTe: Interplay between Dzyaloshinskii-Moriya interaction and higher-order exchange interactions	Megha Arya
	17:40	Study of the microscopic interactions underlying the properties of spin liquids in Kagome lattice of spin 1/2	Flaurent Heully-Alary

Wednesday 9th of October

Chair: Antoine Carof	**09:00**	Gender, biases and prejudice: opportunity or burden?	Florence Sèdes
	09:40	Mechanisms of pyrite formation in marine sediments and implications for isotope fractionation in the presence of trace elements	Jeremy Rabone
	10:00	Modeling biomimetic calcium phosphates using density functional theory	Youness Hajii
	10:20	Structural analysis of the drosophila melanogaster's GSTome	Nicolas Petiot
	10:40	**Coffee break**	
Chair: Carine Clavaguera	**11:00**	Molecular electron density theory study on the mechanism and selectivity of the 1,3 dipolar cycloaddition reaction of N-methyl-C-(2-furyl) nitrone with activated alkenes	Moulay Driss Mellaoui
	11:20	*Ab initio* molecular dynamics calculations on NO oxidation over oxygen functionalized highly oriented pyrolytic graphite	Gilberto Alou
	11:40	Theoretical study of NV centers in diamanes	Samir El Masaoudi
	12:00	Gold fluorocarbenes: Bonding situation and reactivity	Nina Albouy
	12:20	Atomic surface site interaction point model for non-covalent interaction quantification	Katarzyna Zator
	12:40	**Lunch + Posters**	
Chair: Peter Reinhardt	**14:00**	Selected configuration interaction using a transcorrelated Hamiltonian	Anthony Scemama
	14:40	Diving into the continuum with resonances	Yann Damour
	15:00	Probing Quadratic Response for ESA: From Coupled Cluster to TD-DFT	Jakub Sirucek
	15:20	Encodings of vibrational model Hamiltonians on a quantum computer	Joachim Knapik
	15:40	**Closing words and end of JTMS**	

Posters

13:00-13:40 (8th of October)

P1	Hydrogen adsorption and dissociation on impurities covered tungsten surfaces: Classical and Quasi-classical dynamics	Norhan Omar
P2	Hydrogen interaction with W(110) surface	Bombín Raúl
P3	Rotation dynamics of a single Molecule on a Gold Surface by thermal pumping: A semi-classical approach	Afnan Al Saati
P4	Stereodynamics of hydrogen atom scattering off a tungsten surface covered with hydrogen	Raidel Martin Barrios
P5	Structural study and diffusion of lithium in materials for Li$_x$Mn$_{1.5}$Ni$_{0.5}$O$_4$ (LMNO) battery cathodes	Adama Gassama
P6	Theoretical investigation of chiroptical properties of lanthanide complexes	Boris Le Guennic
P7	Theoretical study of NV centers in diamanes	Samir El Masaoudi