Journées Théorie, Modélisation et Simulations - JTMS 2024









Tuesday 8th of October

O9:40 Conceptual theoretical methods to address the challenge of energy density in Li-ion batteries Doublet	_	09:30	Welcome	
10:20 Investigating the effect of particle size and polydispersity on NMR spectra of ions diffusing in disorder porous carbons through a mesoscopic model 10:40 Multi-scale modeling of the dissolution/growth dynamics of metallic copper clusters during synthesis or catalysis processes 11:00 Studying the phase behavior of clay sheets using a flexible coarse-grained model Pauly 11:20 Colloid aggregation simulations at high particle density using fast lubrication dynamics 11:40 Adapting chemical reaction kinetics of biomass fast pyrolysis to fluidized-bed reactor model 12:00 Lunch 13:00 Poster session 13:40 Hydrogen atom scattering from clean and H-covered tungsten surfaces: Recent developments 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 15:00 Modeling multiple photoinduced electron transfers in covalent donor-photosensitizer-acceptor triads 15:20 Neural network-based sum-frequency generation spectra of pure and acidified water interfaces with air 15:40 Dynamics of hydrogen interaction on tungsten surfaces: quantum or classical? 16:00 Coffee break 16:20 Computation of exchange couplings in photogenerated excited states in DFT-KS 16:40 Computation of exchange couplings in photogenerated excited states in DFT-KS 16:40 Computation of exchange couplings in photogenerated excited states in DFT-KS 17:00 Ni surfaces and nanoparticles functionalized with trimethylphosphine: A DFT study of structure sensibility, magnetization and topological analysis 17:20 Prediction of very large skyrmion stability in monolayer MnSeTe: Megha Interplay between Dzyaloshinskii-Moriya interaction and higher-order exchange interactions 17:40 Study of the microscopic interactions underlying the properties of spin Flaurent	ger	09:40	Conceptual theoretical methods to address the challenge of energy	
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liquids in Kagome lattice of spin 1/2 Heully-Alary		17:40	Study of the microscopic interactions underlying the properties of spin	Flaurent
			liquids in Kagome lattice of spin 1/2	Heully-Alary

Journées Théorie, Modélisation et Simulations - JTMS 2024

Wednesday 9th of October

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

Journées Théorie, Modélisation et Simulations - JTMS 2024

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
Р3	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 LixMn $_{1.5}$ 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