Journées Théorie, Modélisation et Simulations - JTMS 2019

Institut de Biologie Physico-Chimique (IBPC, Paris)

Mercredi 5 Juin

09:00	Accueil	
10:00	**Session 1 : Méthodes**	**Boris Le Guennic**
10:00	Mesoscopic simulation of the dynamics of charged species in suspension and in confinement	Marie Jardat
11:00	Study of a new concept of supercapacitors by means of molecular dynamics: biredox ionic liquids	Alessandra Serva
11:20	Towards faster and more stable polarizable dynamics	Félix Aviat
11:40	The moving crude adiabatic representation to avoid conical intersection-related problems in "on-the-fly" quantum dynamics	Loic Joubert-Doriol
12:00	High-throughput solvation free energies by molecular density functional theory and machine learning	Sohvi Luukkonen
12:20	**Déjeuner**	
13:30	**Séance Posters 1**	
14:20	**Session 2 : Méthodes et eau**	**Marie Jardat**
14:20	Nuclear quantum effects in molecules and condensed matter via Quantum Thermal Baths	Fabio Finocchi
14:40	Calculating energy derivatives for quantum chemistry on a quantum computer	Bruno Senjean
15:00	Versatile electrical behavior of 1T-TiS2 elucidated from a theoretical study	Camille Latouche
15:20	Graph-theoretic-based method for conformational search	Sana Bougueroua
15:40	Horizontal & vertical ordering at aqueous interfaces	Simone Pezzotti
16:00	Molecular modeling of nanofluidic systems with slip	Cecilia Herrero
16:20	**Pause café**	
16:40	**Session 3 : Autour de l'eau et des solides**	**Céline Toubin**
16:40	Spéciation du platine en conditions hydrothermales par dynamique moléculaire ab initio	Elsa Desmaele
17:00	Microhydratation of an amphiphile molecule: a step towards the description of clathrate hydrates	Imene Derbali

17:20	DFT study of hydroxyquinoline species as green corrosion inhibitors for aluminum	Yann Bulteau
17:40	Versatile electrification of two-dimensional nanomaterials in water	Benoit Grosjean
18:00	Defects and their influence on the thermoelectric properties of materials: an ab initio study	Philippe Jund
18:20	Relations between electronic structure and properties in solids for energy conversion using the QTAIM approach	Pascal Boulet

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09:00	**Session 4 : Chimie aux interfaces**	**Pascal Larregaray**
09:00	Toward a molecular level investigation of heterogeneous processes for the atmosphere or the interstellar medium	Céline Toubin
10:00	Deposition and thermal processing of interstellar ices: a molecular dynamics study	Pierre Ghesquiere
10:20	Prebiotic organization of biomolecules on mineral surfaces	Hagop Abadian
10:40	**Pause café**	
11:00	**Session 5 : Autour de la bio…**	**Sophie Sacquin-Mora**
11:00	GluT1 mechanism of glucose transport revisited in molecular dynamics study	Tatiana Galochkina
11:20	Elucidation du chemin réactionnel de l'hydrolyse du GTP au sein de petites GTPases	Ruth Tichauer
11:40	QM/MM study of the fluorescence emission of the oxyluciferin and some of its analogues	Madjid Zemmouche
12:00	Simulation of absorption and fluorescence spectra of coloured centers in photochromic sodalites from TD-DFT calculations.	Pauline Colinet
12:20	**Déjeuner**	
13:30	**Séance Posters 2**	
14:20	**Session 6 : Autour des solides**	
14:20	When classical trajectories get to quantum accuracy: the scattering of H_2 on Pd(111)	Alberto Rodriguez-Fernandez
14:40	Wettability@Al_2O_3: Adsorption of lubricants additives by molecular modeling	Sarah Blanck
15:00	How to simulate a montmorillonite mesopore: comparison between Molecular Dynamics force fields and Poisson-Boltzmann	Sébastien Le Crom
15:20	**Pause café**	
15:40	**Session 7 : États excités**	
15:40	Ab initio study of Interatomic Coulombic Electron Capture	Nicolas Sisourat
16:00	Disclosing excited states pathways leading to dual emission using density-based indexes	Anna Perfetto
16:20	New theoretical approaches to study single- and multi-photon processes in atoms and molecules	Eleonora Luppi

Séance poster 1 : 5 Juin

P1-1	Theoretical approaches to get accurate estimates of absorption and emission spectra of aza-BODIPY	Florent Desroches
P1-2	The nucleophilic Reactivity of pyrrolidine: Experimental and theoretical approach	Salma Souissi
P1-3	Electrochemically-assisted Deposition of Sol-Gel Films: Kinetics of Film Growth	Liang Liu
P1-4	RNA synthesis in abiotic conditions: addressing the challenge of phosphoester bond formation	Maud Saint-André
P1-5	Etude mécanistique de la fluoration de s-aryl tétrazines par des complexes de palladium	Pierre Ghesquiere
P1-6	The NCIWEB server for biomolecules: from topological descriptors to binding energies via machine learning	Julia Contreras-Garcia
P1-7	Halogen bond in astatinated R—At...B^- systems	Serigne Sarr
P1-8	Massively parallel implementation of Steered Molecular Dynamics in Tinker-HP: comparisons of polarizable and non-polarizable simulations of realistic systems	Frédéric Celerse
P1-9	Théorie de la fonctionnelle de la densité relativiste à séparation de portée	Julien Paquier
P1-10	Molecular level investigation of the organic/inorganic ions selectivity at the air-liquid interface	Ozge Ozgurel
P1-11	Inelastic Scattering of N_2 off W(001): Reconciling Experiment and Theory at Low Collision Energies	Cesar Ibarguen Becerra
P1-12	A Theoretical Study of Dual Fluorescence in Strap-ESIPT Systems	Amara Chrayteh
P1-13	Heat capacity calculation of mixed-oxide (MOX) fuel using classical molecular dynamics	Didier Bathellier
P1-14	Projected Site-Occupation Embedding Theory	Bruno Senjean
P1-15	Mechanical properties of kaolin group minerals at high pressures: A molecular dynamics study	Brahim Benazzouz
P1-16	Développements théoriques de nouveaux dispositifs de détection de gaz	Mohamed Bensifia
P1-17	Accounting for the metallicity of materials with Thomas-Fermi model in classical molecular dynamics simulations	Thomas Dufils

Séance poster 2 : 6 Juin

P2-1	Structure and solvation in molten carbonates with ab-initio simulation	Antoine Carof
P2-2	Effect of the carbon microporous structures on the capacitance of aqueous supercapacitors	Nidhal Ganfoud
P2-3	Anisotropically corrected Solid-Angle based Nearest-Neighbor algorithm: parameter-free coordination numbers for interfaces	Ruben Staub
P2-4	Molecular basis for thermophoresis in aqueous solutions	Alejandro Diaz Marquez
P2-5	A Density-Based Basis-Set Correction For Wave Function Theory	Emmanuel Giner
P2-6	Modeling interaction of water and methane hydrate with silica surfaces	Konstantin Smirnov
P2-7	Dielectric properties of water and electrolytes at nanometric scale: A field theory approach	Hélène Berthoumieux
P2-8	Getting ions—biomolecules interactions right in Molecular Dynamics simulations	Elise Duboué-Dijon
P2-9	Quasi-Classical Simulation of Resonant Raman Spectra using Linearization in Molecular Dynamics	Hugo Bessone
P2-10	Do concentrated electrolytes exhibit a long range correlation length? A molecular dynamics study	Samuel Coles
P2-11	Molecular simulation of diffusio-osmotic flow profiles	Etienne Mangaud
P2-12	Multi-scale modelling of nano-sensors based on carbon nanotubes (CNTs) and conjugated polymers for water quality monitoring	Robert Benda
P2-13	Réduction du scaling des fluctuations statistiques dans les méthodes de Monte-Carlo Quantiques	Antoine Bienvenu
P2-14	Modeling enzymes orientations on electrode surfaces for green energy production	Nicolas Bourassin
P2-15	On the thermodynamics of crystallization of a confined fluid	Laura Scalfi
P2-16	Formation of Al(8HQ)3 complexes on Al(111) surfaces for the protection of aluminum surfaces against corrosion	Yann Bulteau
P2-17	Hydrogen Activation on Rutile TiO_2 surfaces: A Theoretical study	Baohuan Wei