Journées Théorie, Modélisation et Simulation JTMS 2018

RFCT — DCP — SCF — SCP — GENCI

Salle Jean Jaures, ENS, Paris (entrée par 24 rue Lhomond)

Jeudi 24 mai 2018

09:00 - 10:00 Accueil

10:00 - 12:20 Énergie et Solides (chair Nicolas Sator (Paris))

- 10:00 - 11:00 Multi-scale models to study dynamics and confinement in nanoporous carbons for energy storage applications - Céline Merlet (Toulouse)
- 11:00 - 11:20 H_2 dissociation on CeO_2 surfaces: reducible vs non-reducible - Olivier Matz (Paris)
- 11:20 - 11:40 Electron Transfer in Organic Materials - Antoine Carof (Paris)
- 11:40 - 12:00 Énergie Bleue et désalinisation de l'eau : de la simulation moléculaire aux modèles continus - Nidhal Ganfoud (Paris)
- 12:00 - 12:20 Extracting 3d (Number, Charge And Polarisation)- Densities By Use Of A Reduced Variance Method - Samuel Coles (Paris)

12:20 - 14:00 Pause déjeuner

14:00 - 15:20 Biologie (chair Valérie Brenner (Saclay))

- 14:00 - 14:20 Advancing multi-scale simulation methods for biological membrane systems with applications to confined environments and membrane fusion - Astrid Brandner (Paris)
- 14:20 - 14:40 Effect of Different Activation Methods on CID: Experiments and Chemical Dynamics Simulations on the L-Cysteine Sulfate Anion - Veronica Macaluso (Saclay)
- 14:40 - 15:00 On the effects of learning control in the competition between cancer cells and immune system cells - Leon Masurel (Paris)
- 15:00 - 15:20 AMOEBA Polarizable Force Field Parameters for the HEME Cofactor in the Ferrous and Ferric Forms - Xiaojing Wu (Saclay)

15:20 - 15:40 Pause café

15:40 - 17:00 Solides (chair Annie Lemarchand (Paris))

- 15:40 - 16:00 Predicting auxeticity of zeolitic structures - Romain Gaillac (Saclay)

16:00 - 16:20 Optimization of fluorescence oscillations in a complexation-isomerization system - Agnès Pellissier-Tanon (Paris)

16:20 - 16:40 Exploring the potential energy surface of Ti/SiO_2 nanoparticles - Andi Cuko (Paris)

16:20 - 16:40 GENCI : Présentation des moyens de calcul nationaux - Arnaud Valois (Paris)

17:00 - 17:20 Pause Café

17:20 - 18:20 Électrochimie (chair Claire Lemarchand (Arpajon))

17:20 - 17:40 Finite fields methods for the study of electrochemical systems by molecular dynamics simulations - Thomas Dufils (Paris)

17:40 - 18:00 Molecular Dynamics Simulation Study of Graphene-Based Supercapacitors Combined with Ionic Liquid Electrolytes - Trinidad Méndez Morales (Saclay)

18:00 - 18:20 Étude théorique de "photoswitch" dans des environnements complexes : vers la conception d'actuateurs photoactifs - Laura Le Bras (Paris)

Vendredi 25 mai 2018

09:00 - 10:20 Méthodes (chair Carine Clavaguéra (Orsay))

09:00 - 09:20 Monitoring excited state evolution with the aid of density based indexes - Federica Maschietto (Paris)

09:20 - 09:40 Le Rôle des Indices Basés sur la Densité Électronique dans les Optimisations de Géométries Moléculaires - Juan Sanz Garcia (Paris)

09:40 - 10:00 annulé

10:00 - 10:20 Calculation of potential of mean force: inclusion complexation of azobenzene by calixarenesulfonates and cyclodextrins - Ludovic Garnier (Clermont-Ferrand)

10:20 - 10:40 Pause café

10:40 - 12:20 Catalyse (chair XXX)

10:40 - 11:00 Atomic scattering of H and N on W(100): insights into the differents trapping mechanisms - Cesar Ibarguen Becerra (Bordeaux)

11:00 - 11:20 Mécanismes et sélectivités de la réaction de silylzincation d'alcynes : étude théorique - Frédéric Guégan (Paris)

11:20 - 11:40 Searching for New Borondifluoride Beta-diketonate Complexes with Enhanced Absorption-Emission Properties using ab initio Tools - Miguel Ponce-Vargas (Marne-la-Vallée)

11:40 - 12:00 SFG signals at charged mineral-water interfaces: $\chi(3)(\omega)$ contributions and how to use them for unraveling interfacial structures - Daria Ruth Galimberti (Evry)

12:00 - 12:20 Structure-Properties relationships in substituted, thermoelectric tetrahedrites - Hailong Yang (Marseille)

12:20 - 14:00 Déjeuner

14:00 - 15:20 Méthodes (chair Eric Hénon (Reims))

14:00 - 15:00 Unified formulation of the fundamental and optical gap problems in density-functional theory for ensembles - Emmanuel Fromager (Strasbourg)

15:00 - 15:20 Thermodynamic properties study of $U_{1-y}Pu_yO_2$ MOX fuel using classical molecular Monte Carlo simulation method - Cyrille Takoukam Takoundjou (Marseille)

15:20 - 15:40 Pause café

15:40 - 17:00 Interfaces avec eau (chair Mathieu Salanne (Paris))

- 15:40 - 16:00 Computing the solid/liquid surface tension for anisotropic systems using atomistic simulations - Thibaud Dreher (Clermont-Ferrand)
- 16:00 - 16:20 Accelerating chemical reactions at aqueous interfaces: "on-water" catalysis - Stephanie Essafi (Paris)
- 16:40 - 17:00 Active sieving : from flapping nano-doors to vibrating nanotubes - Sophie Marbach (Paris)

Posters (pendant tout le congrès)

1. Asta Adelchi (Paris) Mesoscopic lattice-based simulations to account for electrokinetics effects and adsorption/desorption
2. Baaden Marc (Paris) Visualisation interactive pour cerner les structures et interactions (macro)moléculaires
3. Benazzouz Brahim (El Harrach, Algérie) Pressure effect on the elastic properties of carbonate MCO_3 : Molecular dynamics study
4. Bourjila Malika (Agadir, Maroc) A Multi Niche Crowding genetic algorithm to generate the Potential Energy Surface of N-formyl-L-alanine-amide
5. Crespos Cedric (Bordeaux) Revisiting dynamics of N_2 on W(100) including van-der-Waals interactions
6. Ferchichi Olfa (Reims) Structural analysis of dioxygen difluoride FOOF
7. Gafour Mohamed Hicham (Relizane, Algérie) DFT and TD-DFT Study of Endohedral Fullerene using Periodic Boundary Conditions
8. Garcia Iriepa Cristina (Marne-la-Vallée) Firefly oxyluciferin and its analogues: simulation and analysis of the spectroscopic properties by QM/MM methods
9. Guillaumont Maya (Paris) Disproportionation or Comproportionation reaction: that is a Computational Chemistry Question
10. Hénin Jérôme (Paris) New developments in adaptive free energy simulations
11. Hénon Eric (Reims) Independent Gradient Model: a new tool derived from the NCI approach to probe strong and weak interactions from wave function calculations or from promolecular electron density
12. Hakiri Rihab (Marne-la-Vallée) The Torsional Dynamics of two conformers of 5-methylfurfural as observed by Microwave Spectroscopy
13. Lemarchand Claire (Arpajon) Algorithme de "polymérisation in situ" en dynamique moléculaire et propriétés dynamiques et structurales de polymères
14. Lesnicki Dominika (Mainz, Allemagne) Increased Acid Dissociation at the Quartz/Water Interface
15. Li Zhujie (Paris) Water Shuttling Mechanisms in Water-in-Salt Electrolytes
16. Luukkonen Sohvi (Paris) High-throughput solvation free energies by molecular density functional theory and machine learning

17. Menicacci Eleonora (Paris) Investigation of ammonium nitrate contaminants based on computational chemistry approaches

18. Mohamed Abd Esselem Dems (Constantine, Algérie) Theoretical study of relation of the electronic properties and RBA in estradiol derivatives

19. Moncomble Aurélien (Lille) Étude théorique et expérimentale de la complexation du cation ZnII avec la morine

20. Morgado Gabriel (Paris) Particle dynamics simulations of Turing pattern in dense systems

21. Nemiche Nardjesse (Oran, Algérie) Study of Density Functional Theory DFT of amphiphilic block copolymer poly(N-vinylpyrrolidone)-b-poly (4-vinyl benzene chloride)

22. Pezzotti Simone (Evry) Hydrophobic aqueous interfaces by DFT-MD simulations and vSFG: 2-Dimentional H-Bond networks

23. Pineau Nicolas (Arpajon) Effets de la granularité lors de la compression sous choc de RDX nanostructuré

24. Rahali Seyfeddine (Nantes) Multi scale study of hydrogen storage on a novel class of Metal Organic Frameworks (MOFs) and Covalent Organic Frameworks (COFs)

25. Ridha Ben Said (Tunis, Tunésie) Étude theorique des mecanismes de la capture du CO_2 par les amines et les diamines primaires et secondaires

26. Sail Karima (Sidi Bel Abbès, Algérie) Structure and Optoelectronic Properties Relationships of Polythiophene: a PBE-DFT and TD-DFT Study

27. Sator Nicolas (Paris) A molecular dynamics perspective on magmas in planetary interiors

28. Schneider Ioan (Le Havre) Collisions réactives des électrons avec des cations moléculaires : dynamique de la fragmentation multi-voies via des états super-excités

29. Siboulet Bertrand (Marcoule) Electro-osmosis : description simple par analyse au niveau moléculaire

30. Soldera Armand (Sherbrooke, Canada) Simulation atomistique de polymères décodée selon un effet caméra ultra-rapide

31. Tanis Ioannis (Arpajon) An anisotropic coarse-grained model of cis-pslybutadiene obtained by a bottom-up approach

32. Treps Laureline (Rueil) Ab initio simulation of the acid sites at the external surface of ZSM-5

33. Wei Baohuan (Paris/Chine) The behaviour of Hydrogen and Deuterium on the Rutile TiO_2 (110) surface : A Theoretical study

34. Zemmouche Madjid (Marne-la-Vallée) Theoretical study of fireflies light emitter and its analogs

35. Zeroual Samira (Batna, Algérie) Étude DFT de ligands pyridines derives de TTF