Monday, 2nd of November

Session 1: Methods (excited states and correlated systems)

13h50 Introduction

14h00 Pierre-François Loos (conférence invitée)
Higher roots of the Schrödinger equation

14h40 David Grégoire
SCF methods for excited states in strong magnetic fields

15h00 Saad Yalouz
A state-averaged quantum algorithm for an equal footing description of ground and excited states on a near term quantum computer

15h20 Sajanthan Sekaran
Quantum embedding for strongly correlated systems

15h40 Mauricio Antonio Rodríguez Mayorga
Improved density matrices from GW approximation

16h00 Posters flash: Mohammad Asad, Christian Brouder, Miguel Escobar Azor, Guillaume Bareigts, Johanna Klein, Richard Asamoah Opoku, Agota Toth, Xiang Yuan, Gaétan Laurens, Mehdi Benmameri

Tuesday, 3rd of November

Session 2: Spectroscopies and interfaces

10h00 Guillaume Le Breton
Second Harmonic Generation at liquid interface: a multi-scale numerical approach

10h20 Juliette Lainé
Molecular understanding of adsorption mechanisms of fatty acids on fluorite under flotation conditions

10h40 Anagha Sasikumar
Relative importance of ring currents and adsorption energies in the determination of in situ NMR spectra

11h00 Roxanne Berthin
The water behavior at electrochemical interfaces: a synergy among molecular dynamics, electrochemistry and Nuclear Magnetic Resonance spectroscopy
11h20  Nawras Abidi  
*Revisiting the active sites on MoS2 in aqueous solution via grand-canonical DFT: The role of water dissociation*

11h40  Paul Clabaut  
*Investigating solvation at metal/water interfaces: the SolvHybrid tool fueled by the GAL forcefield*

**Session 3: Methods (machine learning and various)**

14h00  Julien Lam  
*Gold-Iron interactions in nanoparticles modeled by physically motivated machine learning potential*

14h20  Isaac Chantrenne  
*Discovery of new thermoelectric octahedral transition-metal cluster chalcogenides assisted by artificial intelligence*

14h40  Guillaume Hoffmann  
*Predicting experimental electrophilicities with quantum descriptors: from standard to non linear approaches*

15h00  Miquel Huix-Rotllant  
*Linear scaling electrostatic embedding QM/MM based on electrostatic potential fitted atomic charges*

15h20  Laura Scalfi  
*A semi-classical Thomas-Fermi model to tune the metallicity of electrodes in molecular simulations*

15h40  Pascal Pernot  
*You should not use the mean absolute error to choose a Quantum Chemistry method*

16h00  Posters flash: Mohamed Bensifia, Aimeric Dabin, Théophile Gaudin, Tom Irons, David Lacoste, Roland Panzou, Weiliang Ma, Heng Zhang, Amit Sahu

**Wednesday, 4th of November**

**Session 4: Biology (and molecules of biological interest)**

10h00  Xiaojing Wu (prix Gaston Berthier)  
*Simulation of heme proteins with polarizable force field*
10h40 Olivier Languin-Cattoën
*How do protein conformations define the catch-bond behavior of a bacterial pili?*

11h00 Abderrahmane Semmeq
*DNA under ionizing radiation: The peculiar effect of water*

11h20 Ayoub Daouli
*Tuning the properties of faujasite nanozeolites for optimal capture of O₂/CO₂*

11h40 Mariia Savenko
*Assessing structure and stability of supported lipid bilayers on graphene oxides and silica using all atom molecular dynamics simulations*

**Session 5: Simulations for a variety of applications**

14h00 Arthur Hagopian
*Thermodynamic origin of dendrite growth in metal anode batteries*

14h20 Erika Fallacara
*Order and disorder in KOH and KOD crystals*

14h40 Rabii Larhlimi
*Up to eight nitrogen per bismuth in high pressure BiNₓ phases (x =1-3, 6, 8)*

15h00 Dominika Lesnicki
*Field-dependent ionic conductivities from molecular dynamics simulations*

15h20 Thomas Mangin
*Eu²⁺ extraction to ionic liquids by BTP ligands: Interface crossing studied by MD and PMF simulations*

15h40 Vincent Delmas
*On the reliability of acquiring molecular junction parameters by Lorentzian fitting of I/V curves*

**Thursday, 5th of November**

**Session 6: Spectroscopies (no interfaces)**

10h00 Aurélie Falcone
*Raman spectroscopy for energy materials*

10h20 Aseem Rajan Kshirsagar
*Optical properties of photoresponsive MOFs: assessing fragment models using the BSE/GW formalism*
10h40 Hanna Oher
*A combined ab initio and time-resolved laser-induced fluorescence study of uranium-ligand interactions*

11h00 Manon Bousquet
*Understanding the optical signatures of exotic benzoquinonemonoimine (BQI) \(\pi\)-zwitterions*

11h20 Laurie Lescos
*Performance of DFT functionals for calculating second-order nonlinear optical properties of merocyanine dyes*

11h40 Juan Sanz Garcia
*Unraveling the luminescent pathways of the NanoLuc-furimamide complex*

**Session 7: Reactivity**

14h00 Antoine Geoffroy
*Theoretical study of Diels-Alder Reaction’s asynchronicity with DFT and topological descriptors*

14h20 Radhika Gupta
*Theoretical assessment of “fuzzy” chemical concepts: from chemical bond descriptors to reactivity*

14h40 Gabriel Breuil
*Photo-isomerization of oligo(phenyl-acetylenes) in their first electronic excited states*

15h00 Elise Lognon
*Dihydropyrene photoisomerization mechanism revisited with spin-flip time-dependent density functional theory.*

15h20 Lucien Dupuy
*Quantum cumulative reaction probability in deep tunneling regime from classical-like trajectory simulations*

15h40 Yaidel Toledo-Gonzalez
*Molecular design for catalytic activities of helical chiral oligoureas*

**Friday, 6th of November**

**Session 8: Biology (transport, origin of life)**

10h00 Nathalie Basdevant (conférence invitée)
*Coarse-grained modelling of transport through protein nanopores*
<table>
<thead>
<tr>
<th>Time</th>
<th>Speaker</th>
<th>Title</th>
</tr>
</thead>
<tbody>
<tr>
<td>10h40</td>
<td>Angelika Janaszkiewicz</td>
<td><em>Modeling protein-mediated transport in kidney cells: in silico pharmacology of Organic Anion Transporters</em></td>
</tr>
<tr>
<td>11h00</td>
<td>Mario Rocha</td>
<td><em>Molecular Dynamics simulations of a DNA-based biosensor: How a conformational switch deciphers and predicts the transduction process</em></td>
</tr>
<tr>
<td>11h20</td>
<td>Vishal Kumar Porwal</td>
<td><em>Microscopic understanding of the nanoconfined environment within hybrid layered double hydroxides</em></td>
</tr>
<tr>
<td>11h40</td>
<td>Alejandro Diaz Marquez</td>
<td><em>Molecular basis for thermophoresis in aqueous solutions</em></td>
</tr>
<tr>
<td>12h00</td>
<td></td>
<td><em>Concluding remarks</em></td>
</tr>
</tbody>
</table>