GDR NBODY Workshop

"Electron Many-Body Interactions with Quantum Particles and Fields"

Collège Doctoral Européen, Strasbourg, France, January 15-17, 2025

Organizers: Morgane Vacher (CEISAM, Nantes), Saad Yalouz (LCQS, Strasbourg), and Emmanuel Fromager (LCQS, Strasbourg).

Wednesday, January 15th

Chair: J. Toulouse

13:50 – 14:00 Welcome words, the organizers.

14:00 – 14:50 **Scott M. Garner**, Princeton University, USA. "Dynamics with Nuclear-Electronic Orbital Density Functional and Wavefunction Theories"

14:50 – 15:30 Aurélien de la Lande, Paris-Saclay University, France. "Density Functional Theory Approaches for Ab Initio Modelling of Radiation Chemistry"

15:30 – 15:55 Damian Contant, Sorbonne Université, Paris, France. *"Evaluating nuclear forces with the Optimized Effective Potential approach"*

16:00 – 16:40 **Coffee break**

Chair: M. Vacher

16:40 – 17:20 Jean-Christophe Tremblay, Lorraine University, France. *"Molecular Quantum Dynamics in Stochastic Dissipative Media"*

17:20 – 17:45 Emmanuel Giner, LCT, Sorbonne Université & CNRS, Paris, France. "A Rigorous Density Functional Formulation for QM-MM Problems in the Canonical Statistical Ensemble"

Thursday, January 16th

Chair: E. Fromager

08:40 – 09:35 **Thomas Ebbesen**, ISIS, Strasbourg, France. *"Manipulating Matter by Strong Coupling to the Vacuum Electromagnetic Field"*

09:35 – 10:00 **Lucien Dupuy**, Strasbourg University, LCQS, France. *"Exact Factorization-based Surface Hopping Without Velocity Adjustment: appeal of phase-space formulation for non-adiabatic dynamics"*

10:00 – 10:40 **Coffee break**

10:40 – 11:30 **Federica Agostini**, Paris-Saclay University, France. *"Theory and simulation of ultrafast processes in molecules"*

11:30 – 11:55 Benjamin Bacq-Labreuil, IPCMS, Strasbourg, France. *"Towards an Ab Initio Theory for High-Temperature Superconductors"*

12:15 – 14:00 Lunch at the University restaurant "Le 32"

Chair: S. Yalouz

14:00 – 14:50 **Heiko Appel**, Max Planck Institute, Hamburg, Germany. *"Light-matter interactions within the Ehrenfest-Maxwell-Pauli-Kohn-Sham framework: fundamentals, implementation, and applications"*

14:50 – 15:30 **Rémi Avriller**, LOMA, Bordeaux, France. *"Chirality and Dimensionality in the Ultrastrong Light-matter Coupling Regime: from the Foucault pendulum to the Spyrograph game"*

15:30 – 15:55 Benjamin Tirado, Materials Physics Center, Donostia, Spain. *"Design of quantum circuits to study dissipative processes in plasmonic systems"*

16:00 – 18:00 Poster session and aperitif

Friday, January 17th

Chair: M. Vacher

08:45 – 09:35 Enrico Ronca, Perugia University, Italy. "Strong Light-Matter Coupling by Ab-Initio Methodologies"

09:35 – 10:00 Jérémy Morere, LPCT - CNRS and Université de Lorraine, Nancy, France. "Arbitrariness of the degree of complexity of nested commutators in equation-of-motion formalism"

10:00 – 10:40 **Coffee break**

Chair: L. Dupuy

10:40 – 11:20 **Scott M. Garner**, Princeton University, USA. *"Nuclear-Electronic Orbital Approach for Electronic and Vibrational Polaritons"*

11:20 – 12:00 Johannes Schachenmayer, CESQ, Strasbourg, France. "Dark chemistry in the large-N limit"

12:00 – 12:10 Concluding remarks, the organizers.