

Discussion Meeting force field to study spectroscopic properties

Proposition of Program

Organization: Isabelle Navizet and Etienne Mangaud

For a slot of 1 hour, prepare slides for 30-45 min of talk and allow discussion/questions during the presentation.

For a slot of 30 min, prepare slides for 20 min of talk and allow discussion/questions during the presentation.

Conference will be held at Université Gustave Eiffel, building Lavoisier, RERA Noisy-Champs.

Tuesday 18th April

09:00 – 09:15 Welcome at Plateau K Lavoisier building 3d floor

09:15 – 10:15 Giacomo Prampolini, "Quantum Mechanically Derived Force-Fields: a Tool for Computational Spectroscopy and Material Design"

10:15 – 10:30 Coffee break

10:30 – 11:30 Javier Cerezo,

11:30 – 12:00 Fabrizio Santoro, "Force field driven classical molecular dynamics to investigate environmental effects into the quantum dynamics of nonadiabatic systems"

12:00 – 14:00 Lunch time, Chez Bruno, Hotel Ibis Noisy-Champs

14:00 – 15:00 Carine Clavaguera, "Infrared and vibrational circular dichroism spectroscopy with polarizable force fields"

15:00 – 16:00 Elise Duboué-Dijon

16:00 – 16:30 Coffee break

16:30 – 17:00 Houda Moumene

17:30 – 18:30 Discussion

20:30 Restaurant at L'Européen, Gare de Lyon, 21 bis Boulevard Diderot 75012 paris

Wednesday 19th April

09:00 – 10:00 Jean-Philip Piquemal

10:00 – 11:00 Simon Huppert

11:00 – 11:15 Coffee break

11:15 – 11:45 Thomas Plé

12:00- 14:00 Lunch time, Chez Bruno, Hotel Ibis Noisy-Champs

14:00-14:30 Daniel Roca-Sanjuan (zoom)

14:30-16:00 Discussion: What are the important questions? What are the bottleneck?

Organization of a Workshop/ Summer school in 2024 – 2025?