

## **Programme de la 1/2 journée de l'axe « Théorie et Modélisation » 2023 (jeudi 22 juin)**

**9h15**

"Visualizing a Functional Rare State of Human HSP90 ATP Binding Domain"

**Elisa Rioual**

**9h45**

"Modelling changes of permittivity within charged lipid bilayer stacks by solving a modified Poisson-Boltzmann equation mapped onto Molecular Dynamics simulations"

**Ludovic Gardré**

**10h15**

"Effects of perturbations on a traffic lane"

**Valentin Anfray**

10h40 : coffee break

**11h**

"Approximate range-separated DFT for the band structure of complex materials"

**Thomas Niehaus**

**11h30**

"Developing a potential for clay/organic interactions via a machine learning approach"

**Chloé SANZ**

**12h**

"Understanding transformation-induced plasticity in zirconia ceramics using machine learning potentials"

**Gaël Huynh**

**12h20**

"Multiscale simulations of thermal transport around optically heated heterogeneous nanoparticles in water"

**Julien El Hajj**

12h40 : end of the meeting