

Internship for a Master Student / Stage Master M2 (2025/26)

Topic: Exploring Double Superionicity in Warm Dense Planetary Materials

The interiors of ice giants and many exoplanets contain materials such as **water, ammonia, and methane** compressed to millions of atmospheres and thousands of kelvin. Under these **warm dense matter (WDM)** conditions—where matter lies between the condensed and plasma regimes—ionic and electronic transport phenomena play a crucial role in determining planetary structure, evolution, and magnetic field generation. Recent *ab initio* simulations have predicted the existence of **doubly superionic states**, where **two types of ions become mobile** within a partially ordered lattice. This remarkable behavior, observed in complex H–C–N–O compounds, challenges our current understanding of ion transport and phase transitions in dense plasmas.

This internship aims to test and characterize double superionicity through **first-principles molecular dynamics simulations (DFT-MD)** of selected compounds under planetary interior conditions (300–800 GPa, 2000–8000 K). The project will explore the onset of ion mobility, diffusion mechanisms, and the interplay between structure and charge transport in the WDM regime.

Student tasks

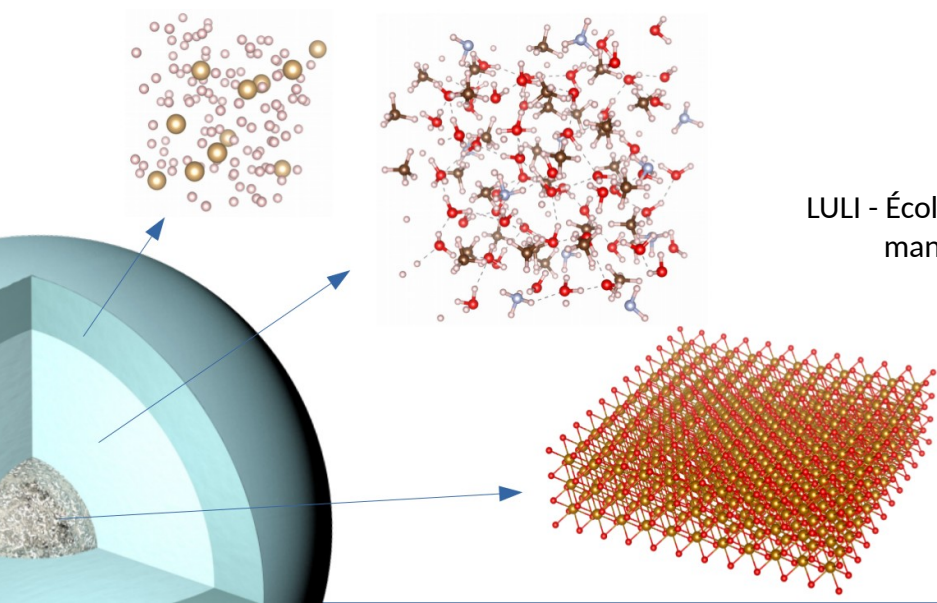
- Perform **DFT-MD simulations** of candidate systems (e.g., $\text{H}_2\text{O}-\text{NH}_3$, HCNO).
- Compute and analyze **diffusion coefficients** and **pair correlation functions** to identify single vs. double superionic behavior.
- Compare results with recent theoretical predictions and discuss implications for **planetary plasmas** and **magnetic field generation**.

Expected profile

- Interest in computational physics, planetary interiors, and/or plasma physics.
- Experience with Linux, Python, and basic simulation tools is a plus.

Expected outcomes

The student will gain hands-on experience in **first-principles modeling of warm dense plasmas** and contribute to testing a novel concept in planetary materials science. The results will help clarify the **physical origin of double superionicity**, an emerging topic at the interface between high-energy-density plasma physics and planetary modeling, and may form the basis for a future publication or PhD project.



Contact

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