INTERNSHIP PROPOSAL

(One page maximum)

Laboratory name:IMPMC
CNRS identification code: UMR7590
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Internship location: IMPMC, Sorbonne University

Thesis possibility after internship: YES
Funding: YES If YES, which type of funding: ANR

Quantum hydrogen storage in ice matrix

Hydrogen-filled ices (HH) represent a fascinating class of quantum materials where hydrogen molecules are confined within a crystalline water framework. Beyond their potential for safe and efficient solid-state hydrogen storage — thanks to high volumetric densities and relatively mild operating conditions — these systems display remarkable quantum phenomena arising from the coupled dynamics of hydrogen and water sublattices.

Recent studies have unveiled hydrogen-rich metastable phases (C0, C2, C3) exhibiting ultra-short H_2–H_2O distances and up to 2:1 H_2:H_2O ratios. In these structures, both the water and hydrogen sublattices participate in a **dual quantum system** in which nuclear quantum effects dominate, driving orientational ordering, hydrogen-bond symmetrization, and lattice symmetry breaking.

The internship will explore **quantum coupling and hydrogen confinement** in these materials using high-pressure and cryogenic techniques combined with **neutron and synchrotron scattering**, supported by path-integral and ab initio simulations. The project will aim to (i) identify new low-pressure synthesis pathways through binary or co-guest systems (e.g. N_2, Ar, THF), (ii) probe the onset of quantum-induced structural transitions, and (iii) establish the microscopic principles enabling dense and recyclable hydrogen storage in expanded ice frameworks.

This research bridges quantum condensed matter physics and energy materials science**,** positioning hydrogen-filled ices as model systems for exploring collective quantum behavior in molecular crystals and for developing quantum-engineered solid hydrogen carriers.

[1] U. L. Ranieri, et al., PNAS 120 (52) e2312665120 (2023). [2] S. DiCataldo, et al., PRL 133 (23), 236101 (2024). (2024). [3] L. Andriambariarijaona, et al. *Physical Review B*, 111(21), 214109 (2025). [4] L. Monacelli, et al. PRB (in press) *arXiv preprint*, arXiv:2506.13169 (2025); [4] L. Renauld et al, submitted arXiv:2510.25707

Please, indicate which speciality(ies) seem(s) to be more adapted to the subject:

Condensed Matter Physics: YES. Soft Matter and Biological Physics: YES
Quantum Physics: YES Theoretical Physics: YES/