Master 2: *International Centre for Fundamental Physics*
INTERNSHIP PROPOSAL

Laboratory name: Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie
CNRS identification code: UMR 7590
Internship director'surname: A. Marco SAITTA – PR
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Internship location: IMPMC – SU – Campus Pierre et Marie Curie
Thesis possibility after internship: YES
Funding: YES If YES, which type of funding: PEPR/Labex/Idex, or ED's

Quantum hydrogen dynamics in ice cages

Gas hydrates, especially hydrogen hydrates, are gaining prominence due to their potential in sustainable technologies like hydrogen storage. Their formation and stability depend on specific temperature and pressure conditions. At different pressures, hydrogen and water crystallize into unique structures, namely the known sII structure and filled ice structures, such as the C_2 one. The microscopic dynamics of guest H_2 molecules within these structures remain largely unexplored.

Inelastic neutron scattering has shown both classical and quantum rotational transitions of H_2 in specific hydrate structures (see Fig.1).

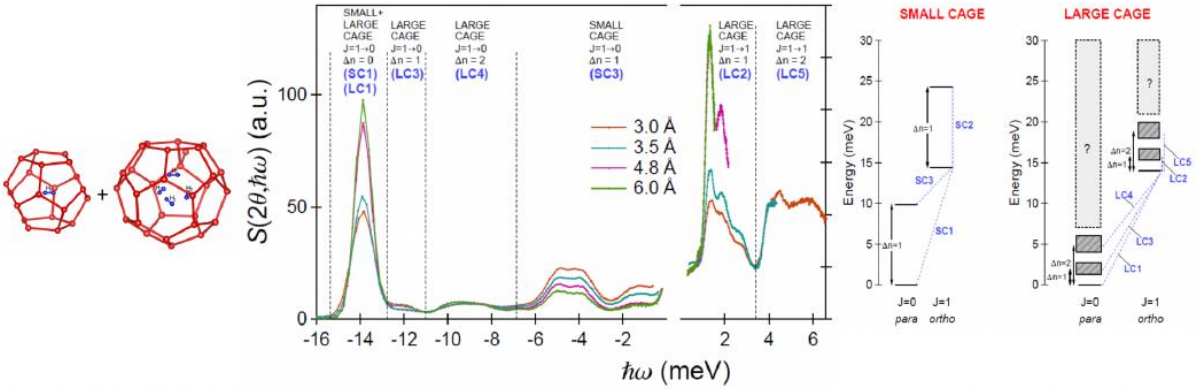

FIG. 1. (left) Small and large cages forming structure sII; (center) INS spectra measured on IN5 at 1.5 K in the sII phase; (right) Measured energy levels for the quantum transitions of the H_2 molecule in the sII phase.

On the other hand, *ab initio* simulations of the high-pressure C_2 structure revealed restricted H_2 molecule rotation at lower temperatures, leading to specific molecular orientations, notably nematic ordering.

Objectives of the internship:

1. Delve deeper into the quantum dynamics that influence H_2 molecule rotation within ice cages, both in classical and quantum rotational transitions.
2. Explore the underlying quantum mechanisms responsible for the observed nematic ordering of H_2 molecules, and establish a connection with observations from Raman light scattering experiments.
3. Develop a machine-learning interaction potential to upscale calculations for larger systems, enhancing our ability to simulate and understand these hydrate systems.

Understanding the quantum dynamics of hydrogen within ice cages will be pivotal for optimizing gas hydrates' properties in sustainable energy storage. The machine-learning potential further ensures that our investigations are scalable, enhancing the applicability and versatility of our findings.

We look for a student willing to undertake these innovative methods and determined to carry out this project within a strong collaboration between theory and experiments. We have a consolidated expertise and a strong publication record including in the last few years, in the theoretical part only, 10 PNAS, 8 PRL, 2 Nature Phys, 3 Nature Comm, 2 Phys Life Rev, 1 Nature Methods, 1 ChemSci.

Techniques/methods in use: quantum path integral dynamics, machine learning, quantum modelling, ab initio molecular dynamics
Applicant skills: strong background in quantum and statistical physics, interest in computational methods, knowledge on machine learning.
Key words: theory, quantum dynamics, statistical mechanics, simulations, machine learning
The supervisor "in action":

Video from my Colloquium at the Physics Department of ENS

Condensed Matter Physics: YES	Macroscopic Physics and complexity: YES
Quantum Physics: YES	Theoretical Physics: YES