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

INTERNSHIP PROPOSAL

(One page maximum)

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Internship location:
Institut des NanoSciences, Sorbonne Université Campus Pierre et Marie Curie
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Thesis possibility after internship: YES
Funding: YES If YES, which type of funding: Sorbonne Center for Artificial Intelligence, Ecole doctorale

Nested Sampling for Nuclear Quantum Effects

Here we propose an internship at the crossing point between applied mathematics and theoretical physics for studying complex quantum phenomena in materials containing light nuclei for which nuclear quantum effects (NQE: zero-point energy, tunneling, etc.) cannot be neglected. We aim at developing machine-learning based techniques for cluster recognition in the nested sampling algorithm to probe complex potential energy surfaces with specific focus to their topology.

The reference methods to study NQE rely on the computationally demanding Feynman path-integrals in conjunction with a thorough configurational space sampling. Potential energy surfaces of interest display several local minima and high dimensionality, which makes most sampling algorithms converge with difficulty. The recognition of cluster structures of the sampling points will be crucial to identify the minima and other relevant extrema. The internship working plan starts with the development of nested sampling including unsupervised cluster recognition to effectively explore classical Lennard-Jones systems, where many local minima are present. Once the specific methods are validated, nuclear quantum effects will be included. The identification and classification of the very many isomers, whose stability can be upset by NQE, is a stringent test for machine-learning methods. Making the most of the experience gained in Lennard-Jones systems, we will implement the methods to cases of high interest in chemistry and physics, such as H-containing clusters and hydrogen diffusion in real materials, where NQE play a significant yet still largely unknown role.

Presently, few groups worldwide are working on the calculation of the quantum free energy by advanced sampling methods that are largely inspired from statistical mechanics. Here, we adopt an original viewpoint, taking advantage of nested sampling with machine learning via cluster recognition to evaluate free energy minima including NQE. This project stems from the conjunction of two complementary skills: one of us (MT) uses cluster recognition methods in nested sampling for Bayesian data analysis; the other (FF) is developing and using several approaches to investigate NQE in several materials. We look for a student with a solid mathematical background, who is motivated by machine-learning applications; a good knowledge of statistical mechanics is a plus.

Techniques involved: Machine learning methods, Nested sampling, Cluster recognition, Feynman path integrals

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

Condensed Matter Physics:	YES	Soft Matter and Biological Physics:	NO
Quantum Physics:	YES	Theoretical Physics:	YES