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

INTERNSHIP PROPOSAL

Laboratory name: **Center for Theoretical Physics of Ecole Polytechnique**
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Thesis possibility after internship: YES
Funding already obtained for a PhD: YES If YES, which type of funding: ANR grant

Elucidating thermal conductivity of high-entropy oxides using machine learning potentials

Understanding the parameters which determine the magnitude of thermal conductivity in solids is of both fundamental and technological interests. Thermal conductivity is sensitive to collective vibrations of atoms in solids that carry energy. Understanding these entropy carriers has led to a number of original phenomena such as the phonon and phonon-electron hydrodynamic regimes in graphite and antimony. In terms of applications, thermal properties of solids are at the heart of major social and environmental issues. For example, the need for highly efficient thermoelectric and thermal barrier devices to save energy has driven the quest for low thermal conductors.

High-entropy alloys, which involve features of both crystalline and amorphous solids, are regarded as a new avenue in search for low thermal conductivity [1,2]. However, due to their highly disordered nature, understanding and predicting their thermal conductivity from first principles calculations is very challenging.

In this master thesis project, which will lead to a fully-funded PhD position, we plan to use machine learning potentials to investigate the thermal conductivity of high-entropy oxides. This will involve evaluating the architecture of available machine learning interatomic potentials, generating the training data using density functional theory calculations, and training the machine learning potentials. Finally, we will use these machine learning potentials in calculating the thermal conductivity and understanding the mechanisms of heat flow.

[1] M.-H. Tsai, Entropy 15, 5338 (2013).
[2] B. Jiang, Y. Yu, J. Cui et al., Science 371, 830 (2021).

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