Machine-learning approaches to model interatomic interactions

Research overview Materials can be studied using computer simulation which enables one to probe the motion of each constituent atoms and to build correlations between the macroscopic properties and the microscopic behaviors. On the one hand, traditional quantum mechanics methods provides particularly accurate results up to the electronic structure of the material. Yet, the drawback of this method concerns its computational cost which prevents from studying large system sizes and long time scales. On the other hand, effective potentials have been developed to mimic atomic interactions thereby reducing those issues. However, these potentials are often built to reproduce bulk properties of the materials and can hardly be employed to study some specific systems including interfaces and nanomaterials. In this context, a new class of interatomic potentials based on machine-learning algorithms is being developed to retain the accuracy of traditional quantum mechanics methods while being able to run simulations with larger system sizes and longer time scales.

Simulation project Using computer simulations, the student will construct a database that should be representative of the different interactions occurring in a specific material. Machine-learning potentials based on the least-angle regression algorithm as well as neural network potentials will be trained and their accuracy will be studied as a function of the size and the complexity of the database.

Supervision and teaching The student will benefit from the supervision of Dr. Julien Lam who is currently *"Chargé de Recherche"* appointed at the Unité Matériaux Et Transformations (Université de Lille). His research is focused on the study of material modeling using many types of computational techniques. The selected student will gain experience in a large number of research domains, especially nanophysics, atomistic simulations, machine-learning and computer programming.

References

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