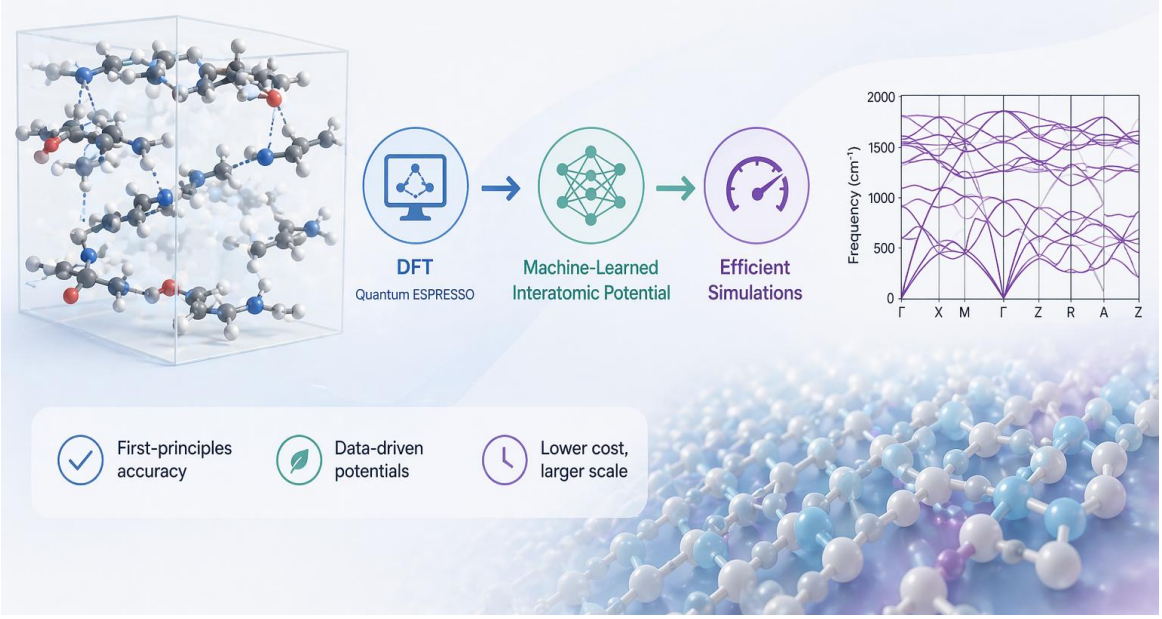
Exploring Molecular Crystals with DFT and Machine Learning



Introduction

Molecular crystals are materials in which weak intermolecular interactions, such as van der Waals forces and hydrogen bonding, strongly affect structural stability, energy, and vibrational properties. Their theoretical description remains challenging, since the results of density functional theory (DFT) calculations depend strongly on the choice of computational parameters, including the exchange–correlation functional, dispersion correction, pseudopotential, and numerical settings.

This project is focused on understanding how different computational approaches influence the predicted properties of molecular crystals. In particular, we will compare DFT-based calculations in Quantum ESPRESSO with a machine-learned interatomic potential (MLIP) in terms of their ability to reproduce equilibrium volume, crystal energy, and phonon spectra. An important part of the work will be to analyze how methodological choices affect the results and what level of accuracy can be expected from different models.

A major goal of the project is not only to teach students how to run calculations, but also to help them understand the theory behind them, including both the physical ideas and the technical details of the computational setup. During the internship, students will learn how such simulations are organized in practice, what types of pseudopotentials are used in Quantum ESPRESSO, and how calculation parameters influence the final results. The project is well suited both for students who would like to try computational materials modeling for the first time and for those who already

have some experience and want to deepen their understanding of atomistic simulations.

Project work

The project is based on atomistic simulations of molecular crystals using Quantum ESPRESSO for DFT calculations and Python scripts for working with a machine-learned interatomic potential (MLIP). Students will learn how to prepare crystal structures, choose pseudopotentials, define the main computational parameters, and organize the calculation workflow from input generation to analysis of the results.

During the project, students will carry out a series of computational studies for selected molecular crystals. This will include structural optimization, calculation of equilibrium volume and total energy, and computation of phonon spectra. They will also perform calculations with the MLIP and compare its results with the DFT data obtained in Quantum ESPRESSO. Particular attention will be paid to the role of methodological choices, such as the type of pseudopotential and the numerical parameters of the calculation, and to how these choices affect the final results.

The final results of the project will be presented in the form of a short report.

Requirements for the student

No strict prerequisites are required. Basic knowledge of physics or chemistry at the university level is expected, including general familiarity with concepts such as atomic structure and intermolecular interactions.

Some experience with programming (preferably in Python) will be helpful but is not mandatory. Prior exposure to computational methods or electronic structure calculations is an advantage, but students without such background are also encouraged to apply.

The main requirement is motivation to learn, readiness to work with computational tools, and willingness to engage with both practical calculations and their underlying theoretical concepts.

Recommended literature

1. **Machine learning interatomic potentials in biomolecular modeling: principles, architectures and applications.**
   Available at:
   https://www.researchgate.net/publication/394420384_Machine_learning_intera

tomic_potentials_in_biomolecular_modeling_principles_architectures_and_applications

2. **Hung, N. T., Nugraha, A. R. T., Saito, R. *Quantum ESPRESSO Course for Solid-State Physics* (2022).**
   A practical introduction to Quantum ESPRESSO, including the basic concepts of DFT and typical computational workflows.
3. **Kittel, C. *Introduction to Solid State Physics*.**
   A classical textbook covering the fundamentals of crystal structure, lattice dynamics, and related physical concepts.

Number of project participants: up to 3

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