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High-throughput screening of adhesive friction in solid-solid interfaces

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First principles high throughput calculations have been successfully applied to screen the properties of hundreds of materials in an automatized way. However, implementing a workflow for high-throughput calculations is challenging and requires robust IT infrastructures to collect, analyze, and save the data. To this end, we have designed and developed an advanced software package to study solid materials with density functional theory (DFT). It allows to carry out high-throughput analyses to evaluate the properties of bulks, surfaces, and interfaces. We used our package to calculate important tribological figures of merit connected to dry adhesive friction of solid-solid interfaces.

Keywords: high-throughput, interfaces, potential energy surface, adhesion, shear strength

1. Introduction

High-throughput studies have become a valuable tool for material advancements, which are of tremendous importance for many industries and closely tied to various societal challenges like clean energy production [1]. To perform an effective high-throughput analysis, it is necessary to develop reliable and scalable software infrastructures. We designed and implemented a workflow to automatize the study of solid crystalline materials with ab-initio DFT calculations. The sotware allows for the investigation of the tribological, mechanical, and electronic properties of bulk crystals, surfaces and interfaces. The workflow is developed modularly and can be easily extended with new modules to calculate additional physical and chemical properties.

2. Methods

Our high-throughput workflows are coded within the FireWorks platform [2] and employ VASP [3] to perform DFT calculations. Starting from two elemental solids, the workflows can generate the surfaces of interest and match them to form an interface, as depicted in Figure 1. The interfacial adhesion, load-displacement curves, shear strength and charge displacements are automatically calculated and the results are stored in a public database.

3. Discussion

In a first application of the high-throughput approach to homogeneous interfaces we generated a database of the shear and cleavage strengths for over hundred interfaces formed by matching two equivalent surfaces of different elemental crystals [4]. We discovered the existence of a power-law between the adhesion and the shear strength for these interfaces. Moreover, the ratio of the strengths can provide an estimate of the material failure mode [5]. The analysis also showed that the mechanical properties of elemental crystals are closely related to their electronic structure [6].
In a more recent advancement, we created a database for heterogeneous interfaces focusing in particular to metal-on-metal surfaces relevant for technological applications and 2D layers adsorbed on solid substrates. The analysis of the overall trends and the comparison of the data obtained for heterogeneous interfaces with the homogeneous counterparts improved the scientific and mechanistic understanding of interface mechanics and tribology [7].

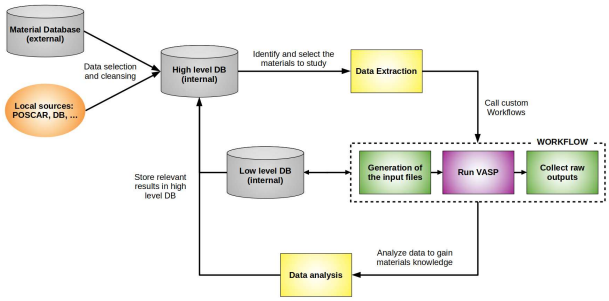

Figure 1: Flowchart of the high-throughput developed by our group.

4. References

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