O 50: Poster Session IV: Tribology: Surfaces and nanostructures II

Time: Tuesday 13:30–15:30 Location: P

O 50.1 Tue 13:30 P

High-throughput ab-initio computation of potential energy surfaces at solid/solid interfaces — •Michael Wolloch[1], Gabriele Losi[2], Omar Chehaimi[3], Mauro Ferrario[2], and M. Clelia Righi[3] — [1]CMP, University of Vienna, Vienna, Austria — [2]FIM, UNIMORE, Modena, Italy — [3]DIFA, University of Bologna, Bologna, Italy

The potential energy surface (PES) characterizes the mechanical properties of an interface to a large extend. It allows the computation of properties like adhesion, shear strength, static friction, and dislocations, among others [1-4]. In the past we have shown that we are able to apply density functional theory to calculate highly accurate PESs for homogeneous interfaces formed by two equivalent surfaces [1,2].

However, the efficient computation of the PES for interfaces consisting of different crystals is exceedingly more complex. Challenges are mainly found in the creation of matching interface structures and the efficient sampling of the interface plane for the total energy calculation.

In this poster we present the algorithm we developed to efficiently and accurately compute the PES of nearly arbitrary interface structures based on the combination of high-symmetry points and interpolation with radial basis functions. A sketch of the full high-throughput workflow is also given.

Part of this work was supported by ERC grant 865633 (SLIDE); [1] Wolloch et al. Sci. Rep. 9, 17062 (2019), [2] Restuccia et al. Comput. Mater. Sci., 154:517-529 (2018), [3] Zilibotti et al. Langmuir 27, 6862 (2011), [4] Mryasov et al. Phys. Rev. B 58, 11927 (1998)

O 50.2 Tue 13:30 P

Nanoscale wear mechanisms on bulk and monolayer molybdenum disulphide — •Alper Özogul[1], Felix Cassin[1], Andrey Turchanin[2], and Enrico Gnecco[1] — [1]Otto Schott Institute of Materials Research, Friedrich Schiller University Jena, Germany — [2]Institute of Physical Chemistry, Friedrich Schiller University Jena, Germany

We have compared the response of MoS2 in the form of multi- and mono-layers grown on a silica substrate under abrasive wear conditions on the nanoscale [1]. The samples have been scratched with a sharp diamond tip with normal loads in the uN range and scan velocities in the um/s range. The resulting surface structures are characterized by AFM and related to the lateral force acting on the probing tip during scratching. On the bulk crystal distinct stick-slip motion is observed and sequences of chip structures are built up all along the scratch line. Characteristic parameters of this motion, namely the lateral contact stiffness and slip period are found to depend highly on the applied normal force and scratching velocity decreasing exponentially or, respectively, increasing logarithmically with them. Monolayer MoS2 is cracked along the zigzag direction and completely folded over itself while scratching. The time evolution of the lateral force is overall irregular although periodic structures, which possibly originate from rippling of silica substrate, can be recognized. First attempts to analyze the energetics of the complex processes so observed are also discussed.

[1] A. Özogul et al., Phys. Rev. Materials 4 (2020) 033603

O 50.3 Tue 13:30 P

Advancing lubricant materials by first principles material design — •Maria Clelia Righi, Stefan Peeters, Gabriele Losi, Michele Cutini, Edoardo Marquis, and Jacopo Mescitelli — Department of Physics and Astronomy, University of Bologna, Italy

Friction and wear result in massive economic and environmental costs. Optimising lubricant materials is challenging because their performances are ruled by molecular-level processes that occur at the buried interface, which are extremely difficult to monitor by experiments. Simulations can play a decisive role here, in particular those based on quantum mechanics, which is essential to accurately describe the interactions between surfaces in contact and simulate reactions in conditions of enhanced reactivity as those imposed by the mechanical stresses applied. We applied ab initio molecular dynamics (MD), also linked to classical MD in a QM/MM scheme, to understand the functionality of lubricant additives and design new, environment-friendly materials to reduce friction. I will describe i) the in-operando formation of graphene from methane molecules ii) iron lubrication by MoS2, phosphorene and selenium-based compounds.

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