O 4: Tribology: Surfaces and Nanostructures

Time: Monday 10:30–12:30 Location: GER 37

O 4.1 Mon 10:30 GER 37

High throughput first-principle prediction of interfacial adhesion energies in metal-on-metal contacts — Paolo Restuccia, •Margherita Marsili, and Maria Clelia Righi — Department of Physics and Astronomy, University of Bologna, 40127 Bologna, Italy

Adhesion energy ultimately dictates the mechanical behavior and failure of interfaces. As natural and artificial solid interfaces are ubiquitous, it represents a key quantity in a variety of fields, from geology to nanotechnology. An *ab-initio* determination of adhesion energies is crucial because the specific atomistic details of the interface primarily determine the strength of adhesion, but, especially for heterogeneous interface is challenging, as computations can be very expensive. We performed the high-throughput DFT determination of the adhesion energy of around a hundred metallic heterostructures, ranging from transition to noble metals [1]. We identified general trends confirming that adhesion energies can be reasonably well inferred from the knowledge of the surface energies of the two interface constituents. Finally, by using a machine learning approach, we obtained a simple analytical expression for predicting the adhesion energy from the intrinsic properties of the two heterostructure constituents alone, which can prove useful for avoiding expensive supercell calculations. These results are part of the SLIDE project funded by the European Research Council under the Horizon 2020 research and innovation program (Grant agreement No. 865633). [1] P. Restuccia et al. *High throughput accurate prediction of interfacial adhesion energies in metal-on-metal contacts* submitted to npj Computational Materials (2022)

O 4.2 Mon 10:45 GER 37

Nanoscale Friction across the First Order Charge Density Wave Phase Transition of 1T-TaS_2 — Wen Wang[1], •Dirk Dietzel[2], and Andrè Schirmeisen[2] — [1]School of Mechanical Engineering, Southwest Jiaotong University, Chengdu, China — [2]Institute of Applied Physics, Justus Liebig University Giessen, Giessen, Germany

In material science, analyzing phase transitions is a fundamental way to understand material properties and their changes on the atomic level. At the same time, phase transition materials are intriguing model systems for nanotribology, where well-defined transformations can occur if a specific control parameter, like e. g. temperature, changes. On one hand, varying friction between tip and sample can be linked to the specific properties of different phases. On the other hand, during the phase transition localized mechanical probing of the surface can allow for a direct coupling to the reorganization of the material as was recently demonstrated for the case of 1T-TaS_2 [1]. However, previous experiments did not allow for an in-depth analysis of the influence of crucial parameters like sliding velocity and normal force on the process of local nucleation. This was now done by friction force microscopy on 1T-TaS2 for different stationary temperatures across the charge density wave phase transitions. Our results corroborate an anticipated mechanism, where the AFM-tip gradually induces local transformations of the material close to the spinodal point in a thermally activated and shear assisted process until the surface is fully 'harvested'.

[1] Panizon et al., New Journal of Physics 20, 023033 (2018).

O 4.3 Mon 11:00 GER 37

Kinetic nanoscale friction on van der Waals heterostructures — •Bartosz Szczefanowicz[1], Zhao Liu[1], Joao Marcelo J. Lopes[2], Antony George[3], Ziyang Gan[3], Andrey Turchanin[3], Alexander Rothstein[4], Christoph Stampfer[4], and Roland Bennewitz[1] — [1]INM - Leibniz Institute for New Materials, Saarbrücken, Germany — [2]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Berlin, Germany — [3]Friedrich Schiller University Jena, Institute of Physical Chemistry, Jena, Germany — [4]JARA-FIT and 2nd Institute of Physics A, RWTH Aachen University, 52074 Aachen, Germany

2D materials exhibit exceptional tribological properties due to their weak normal-to-plane interactions. Friction Force Microscopy (FFM) demonstrated that the microscopic processes underlying friction can be tuned by application of high contact pressure [1] or by combining different 2D materials into van der Waals heterostructures [2].

Samples of $MoSe_2$/hBN and graphene/hBN were prepared by the exfoliation technique. Sample of MoS_2/graphene was produced by thermal decomposition of SiC(0001), followed by direct growth of MoS_2 by Chemical Vapor Deposition (CVD). Friction forces were measured on those heterostructures in FFM experiments in ultrahigh vacuum as function of normal load and electric bias. We will discuss the results in terms of atomic potential corrugation, bending rigidity of 2D heterostructures, and bias-induced electrostatic attraction.

[1] T. Filleter, and R. Bennewitz, Phys. Rev. B, 81, 2010, 155412
[2] M. R. Vazirisereshk, et al., Nano Lett., 19, 2019, 5496-5505

O 4.4 Mon 11:15 GER 37

Temperature Dependent Wear Effects on the Nanometer Scale — •Jennifer Konrad, Dirk Dietzel, and Andre Schirmeisen — Institute of Applied Physics, Justus-Liebig University Giessen, 35392 Giessen, Germany

On the nanoscale, the temperature dependence of friction as observed by friction force microscopy is a well-known phenomenon that can often be described by the thermally activated Prandtl Tomlinson Model. Similarly, nanoscale wear is also often anticipated as a thermally activated and shear assisted process, which results in a temperature dependence, where the overall wear rate increases with temperature [1]. However, this behavior can change when the effects of interfacial bond formation and breaking have to be taken into consideration. Surprisingly, lower temperatures can then result in higher wear rates as will be demonstrated by temperature dependent wear experiments performed for different interfaces involving silica and diamond surfaces. This behavior can phenomenologically be explained by considering shear assisted bond formation, which leads to a higher number of interfacial bonds formed at lower temperatures [2]. By straining this larger number of bonds during scanning an increased wear rate at low temperatures is then caused, even if the energy barrier for bond breaking is lower than for the removal of adjacent surface atoms.

[1] W. Wang, D. Dietzel, and A. Schirmeisen, Phys. Rev. Lett. 126, 196101 (2021).
[2] M. Vorholzer et al., Physical Review X 9, 041045 (2019).

O 4.5 Mon 11:30 GER 37

Rewritable friction on Nitrogen-doped graphene moiré superstructures — •Shuyu Huang[1,2], Antoine Hinaut[2], Yiming Song[2], Sebastian Scherb[2], Gema Gnavarro[2], Thilo Glatzel[2], Yunfei Chen[1], and Ernst Meyer[2] — [1]Jiangsu Key Laboratory for Design and Manufacture of Micro-Nano Biomedical Instruments, School of Mechanical Engineering, Southeast University, Nanjing 211189, China — [2]Department of Physics, University of Basel, Klingelbergstrasse 82, 4056 Basel, Switzerland

Graphene, as typical atomically-thin solid lubricant with potential applications in micro- and nano-electromechanical systems (MEMS/NEMS), has been extensively investigated on its nanotribological properties. In the present work, we compare the frictional properties between pristine graphene and modified graphene, showing that atomic-scale friction can be significantly altered by Nitrogen doping-induced modification, then it can be recovered after tip rubbing. Specifically, C60 nano-flakes are deposited as a mask on graphene/Ir (111) surface by thermal evaporation. The sample is then exposed to a nitrogen radical flux produced by a remote RF plasma source. After thermal annealing, to desorb C60 molecules, both nanopatterned modified graphene and pristine graphene, located below former C60 islands, surface is obtained simultaneously. By the means of high-resolution ultrahigh vacuum atomic force microscopy, the topography of surface with two different regions are characterized and discussed in non-contact mode and friction force variation is measured in contact mode.

O 4.6 Mon 11:45 GER 37

Atomic friction over bonds: Impact of the chemical neighbourhood — •Lukas Hörmann[1], Johannes J. Cartus[1], Alfred J. Weymouth[2], and Oliver T. Hofmann[1] — [1]Institute of Solid State Physics, Graz University of Technology, Graz, Austria — [2]Universität Regensburg, Regensburg, Germany

Friction causes a significant amount of energy loss in any moving mechanical device. Given the trend toward the miniaturisation of devices, studies of the fundamental mechanisms governing friction at the atomic scale become ever more important. At this scale, friction is governed by

electronic and phononic excitations as well as by the potential energy surface (PES) at the interface.

We computationally investigate these mechanisms on the example of a CO-tip of a lateral force microscope oscillating above a PTCDA monolayer on Cu(111). Our investigation combines ab-initio electronic structure methods with machine-learning algorithms to predict highly accurate PESs and to estimate frictional energy dissipation. We gauge the dependence of frictional energy dissipation on the local chemical environment, i.e. the location of the CO-tip above the surface during the friction measurement. Moreover, we investigate how the oscillation direction and the stiffness of the CO-tip affect friction. Hereby we study the role of quantum-mechanical interactions by comparing our results to friction estimates based on a Lennard-Jones potential as well as experimental measurements. Finally, we investigate frictional energy dissipation channels by studying how the movement of the CO-tip may be damped as a result of electronic friction.

O 4.7 Mon 12:00 GER 37

Quantum-mechanically enhanced water flow in sub-nanometer carbon nanotubes — •Alberto Ambrosetti, Giorgio Palermo, and Pier Luigi Silvestrelli — Dipartimento di Fisica e Astronomia, Università degli Studi di Padova, via Marzolo 8, 35131, Padova, Italy

Water-flow in carbon nanotubes (CNT's) starkly contradicts classical fluid mechanics, with permeabilities that can exceed no-slip Haagen-Poiseuille predictions by two to five orders of magnitude. Semi-classical molecular dynamics accounts for enhanced flow-rates, that are attributed to curvature-dependent lattice mismatch. However, the steeper permeability-enhancement observed experimentally at nm-size radii remains poorly understood, and suggests emergence of puzzling non-classical mechanisms. Here we address water-CNT friction from a quantum-mechanical perspective, in terms of water-energy loss upon phonon excitation. We find that combined weak water-phonon coupling and selection rules hinder water-CNT scattering, providing effective protection to water super flow, whereas comparison with a semiclassical theory evidences a friction increase that can exceed the quantum-mechanical prediction by more than two orders of magnitude. Quasi-frictionless flow up to sub-nm CNT's opens new pathways towards minimally-invasive trans-membrane cellular injections, single-water fluidics and efficient water filtration.

O 4.8 Mon 12:15 GER 37

Screw-like beetle joints and their tribological features — •Cornelia F. Pichler[1], Richard Thelen[1], Thomas van de Kamp[2], and Hendrik Hölscher[1] — [1]Institute of Microstructure Technology (IMT), Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Institute for Photon Science and Synchrotron Radiation (IPS), Karlsruhe Institute of Technology, Karlsruhe, Germany

Understanding and finally mimicking lubricants in the joints of various insects promises environmentally friendly alternatives for mineral-oil-based lubricants. The compactness of the insect joints and the tiny quantities of their respective lubricants make it challenging to analyze their frictional properties. In my work, I characterize lubricants directly in dissected screw-like beetle joints by lateral force measurements with the atomic force microscope (AFM). This approach gives insight into the frictional properties of the lubricant in its natural form as well as the functional structure found in the joints. In addition to lubricant films, we also observe microstructures which suggest that beetles advance frictional properties of their joints by a sophisticated combination of surface structure and lubrication.