CPP 42: Friction and Lubrication

Time: Thursday 9:30–11:30 Location: ZEU 114

CPP 42.1 Thu 9:30 ZEU 114

High Resolution Force Measurements of Host-Guest Complex Interaction — •Bianca Bozna[1], Johanna Blass[1,2], Marcel Albrecht[3], Gerhard Wenz[3], and Roland Bennewitz[1,2] — [1]INM - Leibniz Institute for New Materials, Saarbrücken, Germany — [2]Physics Department, Saarland University, Saarbrücken, Germany — [3]Organic Macromolecular Chemistry, Saarbrücken, Germany

Surfaces with well-defined friction and adhesion properties such as high shearing but low peeling resistance are required for many of technical applications. We currently develop a novel surface material based on cyclodextrin assemblies with switchable friction and adhesion characteristics mediated by ditopic guest molecules. As a mandatory step towards achieving this aim, we investigate the friction forces between two surfaces functionalized with β-cyclodextrin in two different configurations. The friction measurements were performed on β-cyclodextrin modified gold surfaces in both pure water and ditopic guest solution (adamantane). The gold surface was functionalized with β-CD molecules whose thiol end groups provide a covalent bond to the substrate. The level of coverage by CD molecules on the gold surface was tested by cyclic voltammetry. Using high resolution friction force measurements we prove that the friction force between the two opposing β-cyclodextrin layers strongly increases in ditopic guest solution when compared to pure water. The long term goal of this research is to develop switchable adherent surfaces that can find applications in biotechnology or medical devices.

CPP 42.2 Thu 9:45 ZEU 114

Structural arrangement of hyaluron and DPPC bilayer under high hydrostatic pressure — •Thomas Zander[1], Florian Wieland[1], Min Wang[2], Akanksha Raj[2], Vasyl Haramus[1], Andra Dedinaite[2], Per Claesson[2], and Regine Willumeit[1] — [1]Helmholz-Zentrum Geesthacht, Institute of Materials Research, D-21502 Geesthacht — [2]KTH Royal Technical Institute, Department of Chemistry, SE-100 44 Stockholm

Articular joints are bio-lubrication systems with the lowest friction coefficients found in nature. The friction coefficient is provided by the synovial fluid, which is an intricate composition of different macromolecules (e.g. phospholipids and hyaluronan) and which keeps the exceptional good lubrication properties even under high loads and shear rates. It is thought that the different constituents form complex structures in order to enable this low friction coefficients.

In order to gain information about the structure of the hyaluronan-phospholipid bilayer samples we performed X-Ray reflectivity measurements at different hydrostatic pressures (1bar - 2kbar). The obtained data clearly reveal the adsorption of hyaluronan to the phospholipid bilayer. Interestingly the structure of the hyaluronan-DPPC layer varies as the molecular weight of hyaluronan is changed. This is supported by DLS and surface-pressure isotherms which show also a stronger interaction with a decreasing molecular weight of hyaluronan.

CPP 42.3 Thu 10:00 ZEU 114

Determining the friction coefficient of a nanometer sized colloid by molecular dynamics simulations — •Zoran Miličević[1], David M. Smith[2,3], and Ana-Sunčana Smith[1,3] — [1]Institut für Theoretische Physik, FAU Erlangen-Nürnberg, Erlangen, Germany — [2]Computer Chemie Centrum, FAU Erlangen-Nürnberg, Erlangen, Germany — [3]Institute Rudjer Bošković, Zagreb, Croatia

Estimation of the transport coefficients of colloids in liquids is still a challenging task for computer simulations. Apart from technical difficulties, the limits of the validity of the Stokes-Einstein relation have not yet been fully established. Here, we calculate the diffusion and the friction coefficients of a nanometer sized particle in water by performing extensive molecular dynamics simulations using the GROMACS software package. We first provide a protocol for defining the hydrodynamic radius of the particle. We then show that both the diffusion and the friction coefficient, and hence the water shear viscosity, can be calculated independently. This is used to demonstrate the validity of the Stokes-Einstein relation in this regime. We compare the obtained results to the shear viscosity calculated independently from pure water simulations and the Green-Kubo relation. We investigate various approaches and present an analysis of simulation conditions required for accurate predictions of transport coefficients, with a particular emphasis on the mass and the size of the spherical particle, as well as the size of the system. As an interesting extension, we study the transport properties of a particle in water subject to a constant electric field, which breaks the otherwise isotropic nature of the system.

CPP 42.4 Thu 10:15 ZEU 114

Switchable friction using asymmetric contacts of stimulus-responsive and non-responsive polymer brushes — •Sissi de Beer[1,2], Edit Kutnyanszky[1], and Julius Vancso[1] — [1]Materials Science and Technology of Polymers, University of Twente, Enschede, the Netherlands — [2]Jülich Supercomputing Centre, Forschungszentrum Jülich, Jülich, Germany

Stimulus responsive (SR), solvated polymers can switch between an expanded and a collapsed conformation via external stimuli. Using molecular dynamics simulations and atomic force microscopy experiments, we show that such SR polymers can be employed to control the frictional response of two opposing polymer brushes in relative sliding motion. By using a brush composed of SR polymers in contact with a non-responsive polymer brush, the overlap between the opposing brushes can be switched ON/OFF: When both brushes are swollen, polymers of the opposing brushes interdigitate, which results in high friction upon shearing. In contrast, when the SR brush is collapsed, the solvent maximizes the interaction with the non-responsive brush. The latter circumvents both brushes from interdigitating, which results in low friction upon shearing.

Invited Talk CPP 42.5 Thu 10:30 ZEU 114

Tribology of colloidal systems — •Clemens Bechinger — Universität Stuttgart, 2. Physikalisches Institut, Stuttgart — Max-Planck-Institut für Intelligente Systeme, Stuttgart

Friction between solids is responsible for many phenomena like earthquakes, wear or crack propagation. Unlike macroscopic objects which only touch locally due to their surface roughness, spatially extended contacts form between atomically flat surfaces. They are described by the Frenkel-Kontorova (FK) model where a monolayer of interacting particles on a periodic substrate potential is considered. In addition to the well-known slip-stick motion the FK-model also predicts the formation of kinks and antikinks which largely reduce the friction between the monolayer and the substrate. Here, we report the direct observation of kinks and antikinks in a two-dimensional charge-stabilized colloidal crystal which is driven across different types of ordered substrates created by interfering laser beams. We show that the tribological properties only depend on the number and density of such excitations which propagate through the monolayer along the direction of the applied force.

- T. Bohlein, J. Mikhael, and C. Bechinger, Observation of kinks and antikinks in colloidal monolayers driven across ordered surfaces, Nature Materials 11, 126 (2012).

- T. Bohlein, and C. Bechinger, Experimental observation of directional locking and dynamical ordering of colloidal monolayers driven across quasiperiodic surfaces, Phys. Rev. Lett. 109, 058301 (2012).

Invited Talk CPP 42.6 Thu 11:00 ZEU 114

Contact and Friction of Rough Adhesive Surfaces — •Mark Robbins[1], Lars Pastewka[1,2], and Tristan Sharp[1] — [1]Johns Hopkins University, Baltimore, Maryland, USA — [2]Fraunhofer-Institut fur Werkstoffmechanik IWM, Freiburg, Germany

Experimental surfaces typically have roughness on a wide range of length scales. This roughness greatly reduces the fraction of the area that is in intimate molecular contact and thus can contribute to friction and adhesion. The talk will first describe recent numerical calculations of elastic contact between rough surfaces with nominally flat or spherical geometries on large scales. An efficient Greens function approach allows calculations for systems with roughness on nanometer to micrometer scales to be performed with atomic resolution in the contact. Results for a wide range of geometries can be collapsed using simple scaling relations that depend on the root mean squared surface slope, sphere radius, elastic modulus, and work of adhesion. The scaling relations explain why adhesive interactions have little effect unless the surfaces are extremely smooth or soft. The traditional Fuller-Tabor model for adhesion of rough surfaces is shown to be qualitatively inconsistent with the simulations. The effect of atomic scale plasticity

on contact and adhesion is surprisingly small. The talk will conclude by considering how forces in the contact area give rise to friction. Friction shows strong scale effects and the partial slip assumed in many contact models is not found in contacts with dimensions of nanometers to micrometers.