

Dissipation Mechanisms in Nano/Mesoscale Tribological Systems | (smr 3713)

Monday, 30 May 2022

08:20 - 08:50 Registration

REGISTRATION: Upon arrival, Visitors not staying in the ICTP Guest Houses, are kindly requested to complete registration formalities in the Leonardo Building Lobby from 8.20 till 8.50 AM CEST.

Location: Leonardo Building (Lobby)

08:50 - 09:00 Opening

Time zone: You can choose your time zone (in place of Europe/Rome) on the top right of the page and the programme time will be modified accordingly

Location: Leonardo Building (Budinich Lecture Hall)

09:00 - 14:20

Location: Leonardo Building (Budinich Lecture Hall)

09:00 **Nanoscale Frictional Behavior of 2D Materials: Connecting Contact Quality and Static Friction 30'**

Speaker: Robert CARPICK (University of Pennsylvania, USA)

Material:  **Video**

09:30 **Fingerprint of a Structural Phase Transition During Superlubric Sliding 20'**

Speaker: Ebru CIHAN (TU Dresden, Chair of Materials Science and Nanotechnology, Germany)

Material:  **Video**

09:50 **Soft and Slippery: Microgel-coated Surfaces under Shear 30'**

Speaker: Carlos Alberto DRUMMOND SUINAGA (Centre de Recherche Paul-Pascal, CNRS, France)

Material:  **Video**

10:20 **Critical Peeling of Tethered Nanoribbons 20'**

Speaker: Andrea SILVA

Material:  **Video**

10:40 **Coffee Break 30'**

11:10 **Magnetic Tuning of Mechanical Dissipation in Quantum Graphene 20'**

Speaker: Alexina OLLIER (University of Basel, Switzerland)

Material:  **Video**

11:30 **Controlled Nanomanipulation and Nanolithography on Mono - and Multilayer MoS₂ Surfaces 30'**

Speaker: Enrico GNECCO (Jagiellonian University, Krakow, Poland)

12:00 **Frictional Properties of Graphene Grain Boundaries: Dynamics of Dislocations and Moiré Superstructures 20'**

Speaker: Xiang GAO (Tel-Aviv University, School of Chemistry, Israel)

Material:  **Video**

12:20 **Translucency and Temperature-dependence for the Slip Length of Water on Supported Graphene - Part 1 30'**

OnLine

Speaker: Ming MA (Tsinghua University, China)

Material:  **Video**

12:50 **Lunch 1h30'**

14:20 - 20:00

Location: Adriatico Guest House (Kastler Lecture Hall)

14:20 **On the Modelling of Triboelectricity and Stress-induced Ionization 30'** (Adriatico Guest House - (Kastler Lecture Hall))

Online

Speaker: Martin MUSER (Saarland University, Saarbrücken)

Material:  **Video**

14:50 **Phonon Transport at Molecular Interfaces – Lessons for Tribologists 30'** (Adriatico Guest House - (Kastler Lecture Hall))

Online

Speaker: Bernd Walter GOTSMANN (IBM Research GmbH, IBM Zurich Research Laboratory, Switzerland)

15:20 **Sliding and Pinning in Superlubric 2D Material Interfaces 20'** (Adriatico Guest House - (Kastler Lecture Hall))

Speaker: Jin WANG (SISSA, Italy)

Material:  **Video**

15:40 **Nanoscale Friction on 2D Materials from Solid Lubrication to Covalent Adhesion 30'** (Adriatico Guest House - (Kastler Lecture Hall))

Speaker: Roland BENNEWITZ (INM - Leibniz Institute for New Materials, Germany)

Material:  **Video**

16:10 **Coffee Break 30'**

16:40 **Sliding Molecules and Mechanical Dissipation Quantum States in Nanoporous Molecular Networks to an Atomic Force Microscope 30'** (Adriatico Guest House - (Kastler Lecture Hall))

Speaker: Remy PAWLAK (University of Basel, Switzerland)

Material:  **Video**

17:10 **New Avenues in Structural Superlubricity: Contact Aging and Friction Switches 20'** (Adriatico Guest House - (Kastler Lecture Hall))

Online

Speaker: Mehmet Zeyyad BAYKARA (University of California Merced, USA)

Material:  **Video**

17:30 **Interfacial Shear at the Atomic Scale 30'** (Adriatico Guest House - (Kastler Lecture Hall))

Online

Speaker: Elisa RIEDO (NYU - Tandon School of Engineering, USA)

Material:  **Video**

18:00 **Poster session (in person) & Welcome reception 2h0'** (Adriatico Guest House - (Kastler Lecture Hall))

All Participants are cordially invited to Welcome Reception at the Adriatico Guest House at 19:00 CEST.

19:00 **Group Photo 5'** (Adriatico Guest House - @ (Terrace))

Tuesday, 31 May 2022

09:00 - 18:00

Location: Leonardo Building - Budinich Lecture Hall

09:00 **The Fascinating Frictional Properties of Layered Materials 30'**

Online

Speaker: Michael URBAKH (Tel-Aviv University, School of Chemistry, Israel)

Material:  **Video**

09:30 **Colloidal AFM Probes Sliding on Graphite: Triboinduced Material Transfer, Atomic-scale Friction and Superlubricity 20'**

Speaker: Renato BUZIO (CNR SPIN, Italy)

Material:  **Video**

- 09:50 **Fluid-electrons Interactions in Carbon Nanomaterials** 30'
 Speaker: Alessandro SIRIA (CNRS ENS, LPS Laboratoire de Physique Statistique, France)
 Material: 
- 10:20 **Energy Dissipation on Twisted Bilayer Graphene at Magic Angle Twist** 20'
 Speaker: Marcin Rafal KISIEL (University of Basel, Switzerland)
 Material: 
- 10:40 **Coffee Break** 30'
- 11:10 **Nature of Dynamic Friction in a Humid Hydrophobic Nanocontact** 20'
 Speaker: Igor STANKOVIC (Institute of Physics Belgrade, Serbia)
 Material: 
- 11:30 **Molecular Nanotribology: Nanomanipulation & Dynamics of Single-Molecules at Surfaces** 30'
 Speaker: Jose Guilherme VILHENA ALBUQUERQUE D'OREY (University of Basel, Switzerland)
 Material: 
- 12:00 **How Adhesion May Interfer in Friction Mechanisms of Viscoelastic Materials?** 20'
 Speaker: Olivier NOEL (CNRS, Laboratory of Physics of Condensed State Materials - LPEC, France)
- 12:20 **Thermal Friction Enhancement in Zwitterionic Monolayers** 30'
 Speaker: Nicola MANINI (Università degli Studi di Milano, Italy)
 Material: 
- 12:50 **Lunch** 1h30'
- 14:20 **Hard Particle Adhesion and on the Stability of Spinning Asteroids** 30'
 Speaker: Bo PERSSON (Forschungszentrum Jülich GmbH, Germany)
 Material: 
- 14:50 **Effects of Friction in Active Matter** 30'
 Speaker: Hartmut LÖWEN (University of Düsseldorf, Germany)
 Material: 
- 15:20 **Rise and Growth of Critical Instabilities in Systems under Shear** 20'
 Speaker: Roberto GUERRA (Università degli Studi di Milano, Italy)
- 15:40 **Plasticity in Nanoscale Friction: Static and Dynamic** 30'
 Speaker: John Bernard PETHICA (Trinity College, Ireland)
- 16:10 **Coffee Break** 30'
- 16:40 **Phase-Transitions in Nano-Friction** 30'

Online

 Speaker: Andre SCHIRMEISEN (Justus-Liebig University Giessen Institute of Applied Physics, Germany)
- 17:10 **Anisotropic Frictional Response of Suspended Graphene** 20'

Online

 Speaker: Andrea MESCOLA (CNR-Istituto Nanoscienze, Italy)
- 17:30 **Atomistic Mechanisms of Friction for MoS2 and Beyond** 30'


Online

 Speaker: Ashlie MARTINI (University of California Merced, USA)
 Material: 

Wednesday, 1 June 2022

09:00 - 18:30

Location: Leonardo Building - Budinich Lecture Hall

- 09:00 **Non-Equilibrium Dynamics and Nanofriction in Ion Coulomb Crystals** 30'
 Speaker: Tanja Elisabeth MEHLSTÄUBLER (Physikalisch-Technische Bundesanstalt & Leibniz Universität Hannover, Germany)
 Material: 
- 09:30 **Markov Dynamics and Entropy Production in a Prandtl–Tomlinson Model** 20'
 Speaker: Alberto PETRI (Consiglio Nazionale delle Ricerche Istituto dei Sistemi Complessi, Italy)

Material:  **Video**

09:50 **Collective Colloidal Dynamics on Ordered and Disordered Landscapes 30'**

Speaker: Pietro TIERNO (University of Barcelona, Spain)

Material:  **Video**

10:20 **Understanding the Rheology of Nanocontacts 20'**

Speaker: Ali KHOSRAVI (SISSA, Italy)

Material:  **Video**

10:40 **Coffee Break 30'**

11:10 **Dissipation and Lubrication of Solid-liquid Nanointerfaces: Complex Balance of Substrate Topography, Molecular Diffusion and Environmental Conditions 20'**

Speaker: Clodomiro CAFOLLA (Durham University, UK)

Material:  **Video**

11:30 **Energy Storage and Dissipation by Forced Wetting and Drying of Nanoporous Materials 30'**

Speaker: Alberto GIACOMELLO (Sapienza University of Rome, Italy)

Material:  **Video**

12:00 **Microscopic Mechanisms of Frictional Aging 20'**

OnLine

Speaker: Wengen OUYANG (School of Chemistry Tel Aviv University, Israel)

Material:  **Video**

12:20 **Unravelling Superlubricity and Interfacial Electrical Contact Mechanism at Single-asperity Level 30'**

OnLine

Speaker: Tianbao MA (Tsinghua University, China)

12:50 **Lunch 1h30'**

14:20 **Moiré-pattern Evolution Couples Rotational and Translational Friction at Crystalline Interfaces 30'**

Speaker: Xin CAO (University of Konstanz, Germany)

Material:  **Video**

14:50 **Open Issues in Pharmaceutical Powders Mechanics 30'**

Speaker: Andrea BENASSI (Chiesi Farmaceutici, Italy)

Material:  **Video**

15:20 **Oscillatory Motion of Viscoelastic Polymer Drops on Slippery Lubricated Surfaces 20'**

Speaker: Matteo PIERNO (University of Padua, Italy)

Material:  **Video**

15:40 **The Nerve Pulse as an Electromechanical Soliton, and How it is Related to Fluctuations and Relaxation Timescales in Biological Membranes 30'**

Speaker: Thomas HEIMBURG (Niels Bohr Institute, University of Copenhagen, Denmark)

Material:  **Video**

16:10 **Coffee Break 30'**

16:40 **Where Did That Charge Come From? 30'**

OnLine

Speaker: Laurence Daniel MARKS (Northwestern University Evanston, USA)

Material:  **Video**

17:10 **Enhancing Liquid/solid Interfacial Energy to Highlight the Elasticity of Mesoscopic Liquids: Long-range Correlations and New Thermodynamic 20'**

OnLine

Speaker: Laurence NOIREZ (Université Paris-Saclay CEA-CNRS, France)

17:30 **Mesoscale Organization in Models of Biological Tissue 30'**

OnLine

Speaker: Maria Cristina MARCHETTI (University of California Santa Barbara, USA)

Material:  Video

18:00 **Poster Session (Virtual) 30'**

Thursday, 2 June 2022

09:00 - 14:30

Location: Leonardo Building - Budinich Lecture Hall

09:00 **Energy Dissipation in Soft Adhesion from a Depinning Perspective 30'**

Speaker: Lars PASTEWKA (University of Freiburg, Germany)

Material:  Video

09:30 **Friction of a Self Assembled Structure at Interface 20'**

Speaker: Seyedmehdi VAEZALLAEI (University of Tehran, Iran)

Material:  Video

09:50 **Grain Boundary Sliding and Low Friction in Metals 30'**

Speaker: Evan Michael CHANDROSS (Computational Materials and Data Science, Sandia National Laboratories, USA)

10:20 **Quantum Theory of Triboelectricity 20'**

Speaker: Alejandro JENKINS VILLALOBOS (International Centre for Theory of Quantum Technologies (ICTQT), Poland)

Material:  Video

10:40 **Coffee Break 30'**

11:10 **Trajectory Anisotropy of a Sliding Tip Induced by Apex Asymmetry 20'**

Speaker: Ali SADEGHI (Shahid Beheshti University, Iran)

Material:  Video

11:30 **Interlayer Electronic Transport in Sheared Bilayer Graphene Systems 30'**

OnLine

Speaker: Elad KOREN (Technion - Israel Institute of Technology, Israel)

Material:  Video

12:00 **Friction, Wear, Lubrication and Tribochemical Reactions Using in Situ Atomic Force Microscopy in Liquids 30'**

OnLine

Speaker: Nitya Nand GOSVAMI (Indian Institute of Technology, India)

Material:  Video

12:30 **Structural Superlubricity: From Dissipation to Functioning 30'**

OnLine

Speaker: Quanshui ZHENG (Tsinghua University Beijing, China)

Material:  Video

13:00 **Lunch 1h30'**

Nanoscale Frictional Behavior of 2D Materials: Connecting Contact Quality and Static Friction

Robert W. Carpick¹

¹ *University of Pennsylvania, Philadelphia, PA, USA 19104*

Two-dimensional materials provide a rich playground for exploring new and unexpected physical phenomena at the atomic limit of thickness. I will focus on friction behavior of nanoscale contacts with 2D materials measured with atomic force microscopy (AFM) and compared with molecular dynamics (MD) simulations. First, nanocontacts with 2-dimensional materials including graphene will be discussed. Friction is far lower than for typical bare substrates, but depends on the number of 2D material layers present. An initial model attributing this to out-of-plane puckering [1] is now enhanced by MD showing a strong role of energy barriers due to interfacial pinning which enhance contact quality, not quantity [2]. We also observe a non-monotonic dependence of friction on humidity for graphite. Using MD, this behavior is attributed to adsorbed water molecules that at low coverage act as pinning sites that enhance contact quality. At high coverage, adsorbates form a quasi-ordered layer that provides a low friction incommensurate interface [3].

We also discuss 2D transition metal dichalcogenides (TMD) including MoS₂. TMDs exhibit intrinsically low friction, although not as low as graphene, which is attributed to the (PES) corrugation [4]. Moreover, friction anisotropy has an unexpected low symmetry, which MD simulations reveal to be due to contact quality effects resulting from the tip's amorphous structure [5]. Finally, we show that varying the chalcogen in MoX₂ (X = S, Se, or Te) leads to an unexpected dependence: instead of the potential energy surface corrugation dominating static friction, the lattice spacing is found to be key; a simple model to explain this result will be presented, and is supported by comparison to the Prandtl-Tomlinson model [6].

[1] C. Lee *et al.* **Science**, 328, 76 (2010). <https://doi.org/10.1126/science.1184167>

[2] S. Li *et al.* **Nature** 539, 541 (2016). <https://doi.org/10.1038/nature20135>

[3] K. Hasz *et al.*, **Phys. Rev. Mat.** 2, 126001 (2018).

<https://doi.org/10.1103/PhysRevMaterials.2.126001>

[4] M. R. Vazirisereshk *et al.*, **Nano Lett.** 19, 5496 (2019).

<https://doi.org/10.1021/acs.nanolett.9b02035>

[5] M.R. Vazirisereshk *et al.*, **J. Phys. Chem. Lett.**, 11, 6900 (2020).

<https://doi.org/10.1021/acs.jpcllett.0c01617>

[6] M.R. Vazirisereshk *et al.*, **ACS Nano**, 14, 16013 (2020). <https://doi.org/10.1021/acsnano.0c07558>

Fingerprint of a structural phase transition during superlubric sliding

Ebru Cihan^{1,2}, Dirk Dietzel¹, and Andre Schirmeisen¹

¹ *Institute of Applied Physics (IAP), Justus-Liebig University Giessen, 35392 Giessen, Germany*

² *Chair of Materials Science and Nanotechnology, Technical University Dresden, 01069 Dresden, Germany (current affiliation)*

Although the fundamental concept of structural superlubricity (i.e. ultra-low friction observed between clean and atomically flat, incommensurate surfaces) is very straightforward, the effective energy barrier for lateral motion still depends on the exact structural dynamics at the sliding interface. In fact, it can be computationally predicted that the superlubricity of amorphous structures is less effective than that of crystalline structures, however this is not always easy to demonstrate experimentally. But we have now overcome this challenge by measuring the friction of antimony nanoparticles on highly oriented pyrolytic graphite in the high temperature regime, i.e. between 300 K and 750 K, where the interface can be restructured. At about 450 K, we trigger a phase transition in antimony nanoparticles, which also allows us to establish a direct link between friction and the interface structure. More specifically, our experiments reveal that the friction level decreases in the more crystalline state where the collective force cancellations are more effective. Due to the irreversible character of the phase transition, a reduced friction level can then also be observed after cooling back to room temperature. The reduction of friction can be associated with a decrease of the characteristic scaling factor γ of about 16%, as theoretically anticipated from the 'scaling law' for superlubricity ($F \propto A^\gamma$)^{1,2}.

[1] D. Dietzel, M. Feldmann, H. Fuchs, U.D. Schwarz, A. Schirmeisen, PRL **111**, 235502 (2013).

[2] E. Cihan, S. Ipek, E. Durgun, M. Z. Baykara, Nat. Comm. **7**, 12055 (2016).

“Soft and slippery: Microgel-coated surfaces under shear”

Pierre Vialar,^{1,2} Suzanne Giasson^{3} and Carlos Drummond^{1,2*}*

1 CNRS, Centre de Recherche Paul Pascal (CRPP), UMR 5031, F-33600 Pessac, France

2 Université Bordeaux, CRPP, F-33600 Pessac, France

3 Department of Chemistry and Faculty of Pharmacy, Université de Montréal, C.P. 6128, succursale Centre-Ville, Montréal, QC, Canada, H3C 3J7

We have investigated the behavior of surfaces coated with dense layers of thermoresponsive pNIPAM-based microgels under compression and shear. We describe how the presence of a long-range repulsive interaction can modify the geometry of approaching surfaces, with significant consequences on normal and friction forces. We show that local surface deformations as small as a few nanometers must be considered to understand the lubrication of the system, in particular when the range of action of normal and friction forces are significantly different. Under these conditions, a subtle interplay between normal forces and surface compliance may significantly reduce friction increment by limiting the minimum approach of the surfaces under pressure. We found that stiffening of compressed microgels confined in the region of closest approach make it increasingly difficult to reduce the gap between the mica surfaces, limiting the contribution of microgels distant from the contact apex to the global friction. In dynamic conditions, we observed the presence of shear-induced lift forces, which can be large enough to entrain a fluid film that separates the surfaces out of contact, driving the dynamic system from conditions of boundary to hydrodynamic lubrication. The origin and consequences of this force will be discussed in detail. These findings suggest simple mechanisms for robust control of lubrication by properly tuning stiffness and geometry of the interacting bodies.

Speaker: Andrea SILVA

Critical Peeling of Tethered Nanoribbons

The peeling of an immobile adsorbed membrane is a well known problem in engineering and macroscopic tribology. In the classic setup, picking up at one extreme and pulling off results in a peeling force that is a decreasing function of the pickup angle. As one end is lifted, the detachment front retracts to meet the immobile tail. At the nanoscale, interesting situations arise with the peeling of graphene nanoribbons (GNRs) on gold, as realized, e.g., by atomic force microscopy. The nanosized system shows a constant-force steady peeling regime, where the tip lifting h produces no retraction of the ribbon detachment point, and just an advancement h of the free tail end. This is opposite to the classic case, where the detachment point retracts and the tail end stands still. Here we characterise, by analytical modeling and numerical simulations, a third, experimentally relevant, setup where the nanoribbon, albeit structurally lubric, does not have a freely moving tail end, which is instead elastically tethered. Surprisingly, novel nontrivial scaling exponents appear that regulate the peeling evolution. As the detachment front retracts and the tethered tail is stretched, power laws of h characterize the shrinking of the adhered length the growth of peeling force and the peeling angle. These exponents precede the final total detachment as a critical point, where the entire ribbon eventually hangs suspended between the tip and tethering spring. These analytical predictions are confirmed by realistic MD simulations, retaining the full atomistic description, also confirming their survival at finite experimental The

Magnetic tuning of mechanical dissipation in quantum graphene

A. Ollier^{1,2}, M. Kisiel¹, R. Pawlak¹, U. Gysin¹, E. Tosatti³, E. Meyer¹

¹*Departement of physics, University of Basel, Klingelbergstrasse 82, 4056 Basel (CH)*

²*Swiss Nanoscience Institute, Klingelbergstrasse 82, 4056 Basel (CH)*

³*SISSA, Trieste, Via Bonomea 265, Italy*

(Corresponding author: A. Ollier, email: alexina.ollier@unibas.ch)

Understanding nanoscale energy dissipation is nowadays among few priorities particularly in solid state systems. Breakdown of topological protection, loss of quantum information and disorder-assisted hot electrons scattering in graphene are just few examples of systems, where the presence of energy dissipation has a great impact on the studied object [1]. It is therefore critical to know, how and where energy leaks. Pendulum geometry Atomic Force Microscope (pAFM), oscillating like a pendulum over the surface, is perfectly suited to measure such tiny amount of dissipation [2,3], since a minimum detectable power loss is of the order of aW.

We report on a low temperature ($T=5\text{K}$) measurement of striking singlets or multiplets of dissipation peaks above graphene nanodrums surface. The structure geometry leads to formation of few nanometre size graphene wrinkles and the observed dissipation peaks are attributed to tip-induced charge states transitions in quantum-dot-like entities. The dissipation peaks strongly depend on the external magnetic field ($B=0\text{T}-2\text{T}$). The magnetic field induce Peierls phase that shift the peaks to lower energy. At large magnetic field this shift induces the vanishing of the peaks.

[1] D. Halbertal, *et al.*, Nanoscale thermal imaging of dissipation in quantum systems, *Nature* **539**, 407-410(2016)

[2] B. C. Stipe, *et al.*, Noncontact friction and force fluctuations between closely spaced bodies, *Phys. Rev. Lett.* **87**, 096801(2001)

[3] M. Kisiel, *et al.*, Suppression of electronic friction on Nb films in the superconducting state, *Nature Materials* **10**, 119-122(2011)

Controlled nanomanipulation and nanolithography on mono- and multilayer MoS₂ surfaces

**Enrico Gnecco^{*1}, Felix Cassin², Alper Özogul³, Arkadiusz Janas¹, Benedykt R. Jany¹
and Franciszek Krok¹**

¹*M. Smoluchowski Institute of Physics, Jagiellonian University, Krakow, Poland*

²*M Advanced Research Center for Nanolithography (ARCNL), Amsterdam, The Netherlands*

³*Institute of Materials Science, Technical University Dresden, Germany*

Due to their superlubric properties and their wear resistance, MoS₂ surfaces are very attractive for applications and fundamental investigations in nanotribology.

In the first part, we will present a series of experiments on the collective manipulation of metal clusters on mono- and multilayer MoS₂ surfaces as performed by AFM under ambient conditions. Starting with a general equation that relates the direction of motion of spherical particles to the scanning pattern, the influence of friction on the manipulated particle trajectory fluctuations, and the influence of particle shape on the manipulation process will be introduced. Atomic-scale effects become important when the cluster and substrate form commensurable contacts, as for triangular Au clusters on MoS₂ [1]. In this case we observed a preferential motion along the zigzag direction of the substrate regardless of the moment imparted by the AFM tip. The formation of long Au stripes parallel to the fast scan direction is also an important effect observed when the cluster density is sufficiently high, albeit hampered by the corrugation of the underlying SiO₂ substrate [2].

In the second part, we will discuss the formation of wear nanostructures from AFM lithography on mono- and multilayer MoS₂. A typical result is the detachment of flakes with crack propagation along the zigzag direction of the MoS₂ lattice [3]. On a monolayer, nanoexfoliation is also accompanied by surface rippling of the silica substrate [4]. This will lead to a final digression on the formation of wavy patterns on (non-layered) surfaces, which we are also attempting to model based on the frictional stick-slip accompanying the wear process.

[1] F. Trillitzsch, R. Guerra, A. Janas, N. Manini, F. Krok, E. Gnecco, *Phys. Rev. B* **98**, 165417 (2018)

[2] F. Trillitzsch, A. Janas, A. Özogul, C. Neumann, A. George, B.R. Jany, F. Krok, A. Turchanin, E. Gnecco, *MRS Advances* **5**, 2201 (2020)

[3] A. Özogul, E. Gnecco, M.Z. Baykara, *App. Surf. Sci. Adv.* **6**, 100146 (2021)

[4] A. Özogul, F. Trillitzsch, C. Neumann, A. George, A. Turchanin, E. Gnecco, *Phys. Rev. Materials* **4**, 033603 (2020)

Frictional Properties of Graphene Grain Boundaries: Dynamics of Dislocations and Moiré superstructures

Xiang Gao¹, Oded Hod¹, and Michael Urbakh¹

¹ *Department of Physical Chemistry, School of Chemistry, The Raymond and Beverly Sackler Faculty of Exact Sciences and The Sackler Center for Computational Molecular and Materials Science, Tel Aviv University, Tel Aviv 6997801, Israel.*

Van der Waals homo- and heterojunctions formed by two-dimensional (2D) layered materials own tremendous potentials in structural superlubricity, which has been demonstrated by experiments up to microscale [1-3]. Aiming to achieve structural superlubricity at increasing length scales, unavoidable grain boundaries (GBs) should be considered as energy barriers introduced due to topographic distortions lead to additional energy dissipation. Meanwhile, at a heterogeneous layered interface (e.g. *h*-BN/polycrystalline graphene (PolyGr)) or an incommensurate (e.g twisted) homogeneous interface, moiré superstructures naturally appear in the reconstructed lattice, rendering well-defined domains and domain walls, where tensile and compressive in-plane stresses accumulate. In the presence of GBs, the collective motion of moiré superstructures are strongly restricted, resulting in their reflection, annihilation, or creation at the GBs. This, in turn, involves intricate strain accumulation and release processes that generate additional interfacial energy dissipation, leading to unique unexplored frictional behaviors.

Using state-of-the-art force field simulations, we investigated the frictional properties of graphene GBs in finite and infinite, homo- and heterojunctions [4-6]. Depending on the GB misfit angle, the topological defects along typical GBs can vary from being nearly flat to highly corrugated. For corrugated GBs, the kinetic friction is found to be dominated by shear induced buckling and unbuckling, leading to a nonmonotonic behavior of the friction with normal load and temperature. The underlying mechanism involves two effects, where an increase of dislocation buckling probability competes with a decrease of the dissipated energy per buckling event. These effects are well captured by a phenomenological two-state model. The resulting negative differential friction coefficients can reduce the expected linear scaling of GB friction with surface area and restore structural superlubricity at increasing length-scales.

In addition, we demonstrated for *h*-BN/PolyGr heterojunction a new frictional mechanism based on collective stick-slip motion of moiré superstructures in normal load regime. The dissipative stick-slip behavior originates from an energetic bi-stability between low- and high-commensurability configurations of large-scale moiré superstructures. The discovered phenomenon is expected to be of general nature and occur in many other large-scale layered material interfaces.

[1] O. Hod, E. Meyer, Q. Zheng, and M. Urbakh, *Nature* **563**, 485 (2018).

[2] Y. Song, D. Mandelli, O. Hod, M. Urbakh, M. Ma, and Q. Zheng, *Nat. Mater.* **17**, 894 (2018).

[3] M. Liao, P. Nicolini, L. Du, J. Yuan, S. Wang, H. Yu, J. Tang, P. Cheng, K. Watanabe, T. Taniguchi et al., *Nat. Mater.* **21**, 47–53 (2022).

[4] X. Gao, W. Ouyang, O. Hod, and M. Urbakh, *Phys. Rev. B* **103**, 045418 (2021).

[5] X. Gao, W. Ouyang, M. Urbakh, and O. Hod, *Nat. Commun.* **12**, 5694 (2021).

[6] X. Gao, O. Hod, and M. Urbakh, submitted.

Translucency and temperature-dependence for the slip length of water on supported graphene

Han Li^{1,2}, Zhi Xu^{1,2}, Chen Ma^{2,3}, Ming Ma^{1,2*}

¹Department of Mechanical Engineering, State Key Laboratory of Tribology, Tsinghua University, Beijing 100084, China

²Center for Nano and Micro Mechanics, Tsinghua University, Beijing 100084, China

³Department of Engineering Mechanics, Tsinghua University, Beijing 100084, China

Abstract

Carbonous materials, such as graphene and carbon nanotube, have attracted tremendous attention in the fields of nanofluidics due to the slip at the interface between solid and liquid. The dependence of slip length for water on the types of supporting substrates and thickness of carbonous layer, which is critical for applications such as sustainable cooling of electronic devices, remains unknown. In this paper, using colloidal probe atomic force microscope, we measured the slip length of water on graphene supported by hydrophilic and hydrophobic substrates, i.e., SiO₂ and octadecyltrimethoxysilane (OTS). The slip length l_s on single-layer graphene supported by SiO₂ is found to be 1.6 ± 1.9 nm, and by OTS is 8.5 ± 0.9 nm. With the thickness of few-layer graphene increases to 3~4 layers, both l_s gradually converge to the value of graphite (4.3 ± 3.5 nm). Such thickness dependence is termed slip length translucency. Further, l_s is found to decrease by about 70% with the temperature increases from 300 K to 350 K for 2-layer graphene supported by SiO₂. These observations are explained by analysis based on Green-Kubo relation and McLachlan theory. Our results provide the first set of reference values for the slip length of water on supported few-layer graphene. They can not only serve as a direct experimental reference for solid-liquid interaction, but also provide guideline for the design of nanofluidics-based devices, for example the thermo-mechanical nanofluidic devices.

Keywords: water, graphene, slip length, atomic force microscope

On the modelling of triboelectricity and stress-induced ionization

Martin H. Müser and Sergey Sukhomlinov

Dept. of Materials Science and Engineering, Saarland University, Germany

Triboelectricity is one of the best and longest-known natural phenomena. While charge-transfer between metals can be said to be well understood, there is an ongoing debate as to the relevant charge-transfer mechanism for dielectrics rubbing against each other. Various experiments have been conducted and interpreted to be clearly in favour of either electron transfer or ion transfer, without coming to an agreed-upon, general mechanism. The modelling community has remained surprisingly silent. One of the difficulties may be that in order to model electronic charge transfer, systems can no longer be assumed to be in their electronic ground state. This causes tremendous difficulties for density-functional theory (DFT) based approaches. However, classical potentials can overcome this bottleneck [1], as will be presented in this talk. DFT can nevertheless be used to model stress-induced ionization. We find bulk systems containing various phosphor-containing molecules to ionize under pressures as small as 1 GPa when sufficiently sheared. The considered conditions are yet quite moderate for tribological contacts. Simply heating the systems only induces zwitterions but not free ions.

[1] W. Dapp and M. H. Müser, *Eur. Phys. J. B* **86**, 337 (2013).

[2] S. V. Sukhomlinov, G. Kickelbick, and M. H. Müser, *Tribol. Lett.* (submitted).

Phonon Transport at Molecular Interfaces – Lessons for Tribologists

Bernd Gotsmann

IBM Research Europe - Zurich

The phononic coupling of molecules governs tribological and thermal transport properties. Phonon coupling properties can be assessed through thermal transport measurements. However, at small length scales the measurement has been a challenge to the experimentalist. Recently we have measured thermal transport through single molecules for the first time [1] and we will discuss the results in terms of heat transfer models, Wiedemann Franz law, coherence and localization. Instead of considering local vibrations at the various degrees of motion of a molecule at a surface, it is useful to rationalize the vibrations as ingredients to a scattering problem of propagating phonons. Thereby a link between the fields of thermal transport and tribology can be made. This talk will have tutorial style elements and include discussion on open questions and opportunities for both fields.

[1] N. Mosso, H. Sadeghi, A. Gemma, S. Sangtarash, U. Drechsler, C. Lambert, B. Gotsmann, “Thermal Transport through Single-Molecule Junctions”, Nanoletters 2019, <https://pubs.acs.org/doi/10.1021/acs.nanolett.9b02089>

This work has also received funding from the Swiss National Science Foundation with project no. 200660 and from the European Commission H2020-FETOPEN projects ‘EFINED’, grant agreement no. 766853, and ‘QuIET’, grant agreement no. 767187.

Sliding and Pinning in Superlubric 2D Material Interfaces

Jin Wang¹ , Ali Khosravi^{1,2,3} , Andrea Vanossi^{3,1}, and Erio Tosatto^{1,2,3}

¹*International School for Advanced Studies (SISSA), Via Bonomea 265, 34136 Trieste, Italy*

²*The Abdus Salam International Centre for Theoretical Physics (ICTP), Strada Costiera 11, 34151 Trieste, Italy*

³*CNR-IOM, Consiglio Nazionale delle Ricerche - Istituto Officina dei Materiali, c/o SISSA Via Bonomea 265, 34136 Trieste, Italy*

Graphene and many other 2D materials entered the physics and engineering scene in the last two decades. Their strong and yet membrane-like sheets permit – actually require -- deposition, giving rise to interfaces whose tribological properties under shear stress must be understood and controlled. We carried out selected simulation case studies with variously twisted, structurally lubric interfaces involving graphene. There is first of all a basic difference between "small" and "large" twist angles -- only the latter are structurally lubric and free sliding in the usual sense. The kinetic friction of a superlubric sliding island is linear with velocity ("viscous") at large velocity or large temperature -- regimes where, dominated by the island's body, friction grows proportional to area. At low velocities and low temperatures, conversely, kinetic friction is, like static friction, dominated by the edges of the island. Therefore growing at most as the perimeter, and with a much weaker velocity dependence, as expected for stick-slip friction. Recovering and extending many results already present in literature, the overall picture obtained applies to general 2D interfaces, including current and future bilayer and multilayer systems.

Nanoscale friction on 2D materials – from solid lubrication to covalent adhesion

Bartosz Szczefanowicz, Zhao Liu, Günther Krämer, Roland Bennewitz
INM – Leibniz-Institute for New Materials, Saarbrücken, Germany

Takuya Kuwahara, Leonhard Mayrhofer, Andreas Klemenz, Michael Moseler
Fraunhofer Institute for Mechanics of Materials IWM, Freiburg, Germany

Two-dimensional materials such as graphene or MoS₂ offer interesting tribological perspectives. Their strong in-plane cohesion and weak out-of-plane interaction favor sliding at low dissipation. We will discuss three force microscopy experiments which address microscopic mechanisms of friction on 2D materials.

Alkane lubricants are known to exhibit an ordered layering when confined to nanometer-scale gaps. We found that this effect is greatly enhanced when a steel surface is covered by a monolayer of graphene, bringing about a significant increase in load-bearing capacity of the oil layer. [1]

Friction force experiments on epitaxial graphene/SiC(0001) have demonstrated ultralow friction [2]. However, friction increases abruptly and irregularly when the pressure under the AFM tip reaches values of about 7 GPA. We attribute this friction increase to the formation of covalent bonds between graphene and substrate, essentially a sp²-to-sp³ transition under pressure. The experimental results can be understood in terms of bond formation as simulated by DFT and tight-binding methods.

Nanoscale friction on MoS₂ depends on the number of layers. The underlying mechanisms are investigated by varying load and applied electrical bias. The results reveal that adhesion and shear strength have to be considered in the description of friction of multilayer MoS₂ on graphene/SiC(0001).

[1] G. Kramer, C. Kim, K.S. Kim, R. Bennewitz, Single layer graphene induces load-bearing molecular layering at the hexadecane-steel interface, *Nanotechnology*, 30 (2019).

[2] T. Filleter, J.L. McChesney, A. Bostwick, E. Rotenberg, K.V. Emtsev, T. Seyller, K. Horn, R. Bennewitz, Friction and Dissipation in Epitaxial Graphene Films, *Phys. Rev. Lett.*, 102 (2009).

Sliding Molecules and Mechanical Dissipation Quantum States in Nanoporous Molecular Networks to an Atomic Force Microscope

Rémy Pawlak¹, Philipp D'Astolfo¹, Xunshan Liu², Ulrich Aschauer², Silvio Decurtins², Shi-Xia Liu², and Ernst Meyer¹

¹*University of Basel, Department of Physics, Klingelbergstrasse 82, Basel, 4056, Switzerland*

²*Department of Chemistry and Biochemistry, University of Bern, Freiestrasse 3, 3012 Bern Switzerland*

Periodic confinement of surface electrons in atomic structures or extended nanoporous molecular networks is the archetype of a two-dimensional quantum dot (QD) superlattice [1]. Yet, an electrical control of such an artificial lattice by external gating has never been demonstrated. In work, we show the mechanical coupling between an atomic force microscope (AFM) and quantum states engineered in highly crystalline nanoporous molecular networks on Ag(111). We characterize local density of states (LDOS) using scanning tunneling microscopy (STM). Low-temperature force spectroscopy reveals force/dissipative responses at threshold voltages that arise from charging/discharging of the superlattice's eigen-states under the local electric field of the tip. We infer the quantum capacitance and resonant tunneling rates, opening new avenues in the characterization of exotic phenomena in designer quantum materials via a nanomechanical oscillator.

[1] M. F. Crommie, C.P. Lutz, and D.M. Eigler. *Science* **262**, 218–220 (1993).

[2] P. D'astolfo *et al.* Submitted.

New Avenues in Structural Superlubricity: Contact Aging and Friction Switches

Wai H. Oo¹ and Mehmet Z. Baykara¹

¹Department of Mechanical Engineering, University of California Merced, USA

We present results of nanomanipulation experiments performed on gold nanoislands on graphite, a material system that exhibits structural superlubricity under ambient conditions [1]. Utilizing the “tip-on-top” manipulation approach [2], we reveal previously undiscovered effects in structural superlubricity: (i) significant contact aging and (ii) spontaneous jumps (i.e. *switches*) between high and low friction *branches* (Figure 1). Repeated experiments conducted with islands of different size and under different environmental conditions point toward a strong influence of contact size and sample contamination on both effects, indicative of a non-trivial interplay between interface structure and chemistry affecting energy dissipation mechanisms in this elusive ultra-low friction regime.

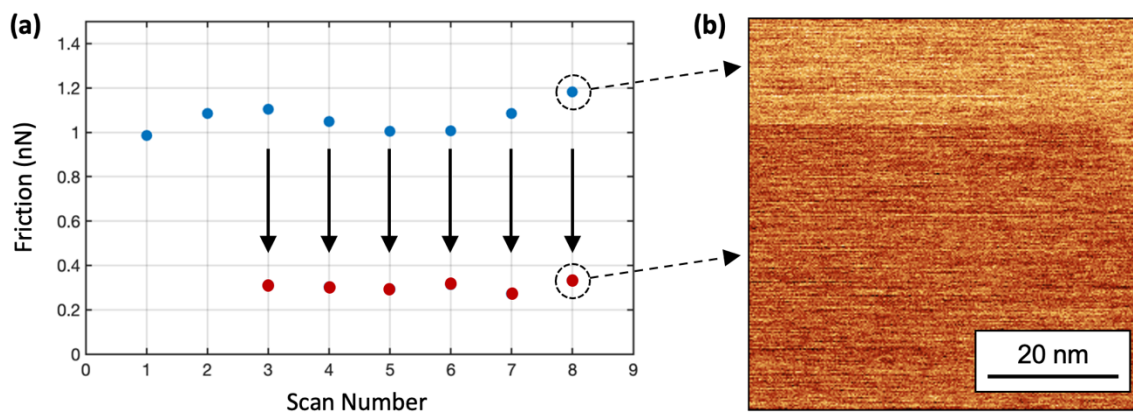


Figure 1. (a) Mean friction force recorded during the repeated manipulation of a single gold nanoisland on graphite, as a function of scan number. Black arrows indicate switches from the high (blue dots) to low (red dot) friction branch that occur in an individual scan. (b) Friction force map recorded during Scan 8, whereby a high and low friction regime can be clearly distinguished.

[1] E. Cihan, S. Ipek, E. Durgun, M.Z. Baykara, Nat. Commun. **7**, 12055 (2016).

[2] D. Dietzel, M. Feldmann, H. Fuchs, U.D. Schwarz, A. Schirmeisen, Appl. Phys. Lett. **95**, 053104 (2009).

Interfacial Shear at the Atomic Scale

Martin Rejhon, [Elisa Riedo](#)

Tandon School of Engineering, New York University, Brooklyn, NY, 11201, USA

Two-dimensional (2D) materials, such as graphene, are usually exfoliated onto, or directly grown on a substrate. Since 2D films or flakes are only one or a few atoms thick, their interaction with the substrate is of key importance. Indeed, substrate and interlayer interaction can change 2D materials chemical [1-2], mechanical [1-2], and electronic properties [3]. From Fermi level pinning to strain engineering, phase transitions, and superlubricity, understanding the interfacial properties between an atomic layer and its substrate is of great interest at both the fundamental and technological level.

Here, we measure the hardly accessible interfacial transverse shear modulus of an atomic layer on a substrate [4]. By performing measurements on bulk graphite, and epitaxial graphene films on SiC with different stacking order and twisting, as well as in presence of intercalated hydrogen between graphene and SiC, we find that the interfacial transverse shear modulus is critically controlled by the stacking order and the atomic layer-substrate interfacial interaction. Importantly, we also demonstrate that this modulus is a pivotal measurable property to control and predict sliding friction in supported two-dimensional materials. Indeed, we observe a novel general reciprocal relationship between the friction force per unit contact area and the interfacial shear modulus for all the investigated graphitic structures, including twisted graphene and bulk graphite. This relationship is supported by simple friction models based on a point mass driven over a periodic potential, where the atomic layer-substrate interaction controls the shear stiffness and therefore the resulting friction dissipation.

[1] Gao, Y., et al. (2018). "Ultrahard carbon film from epitaxial two-layer graphene." *Nature Nanotechnology* **13**(2): 133-138, doi:10.1038/s41565-017-0023-9

[2] Cellini, F.; Lavini, F.; Berger, C.; de Heer, W.; Riedo, E., (2019) "Layer dependence of graphene-diamene phase transition in epitaxial and exfoliated few-layer graphene using machine learning". *2D Materials*, 6 (3), doi:035043 10.1088/2053-1583/ab1b9f

[3] Zheng, X. R.; et al., Patterning metal contacts on monolayer MoS₂ with vanishing Schottky barriers using thermal nanolithography. *Nature Electronics*, 2 (1), 17-25, doi:10.1038/s41928-018-0191-0

[4] Martin Rejhon, Ali Khosravi, Erio Tosatti, Elisa Riedo (2022) "Interfacial Shear at the Atomic Scale", under revision.

The fascinating frictional properties of layered materials

Michael Urbakh

School of Chemistry, Tel Aviv University, Tel Aviv 6997801, Israel

Tribology - the science of friction, wear, and lubrication - is of fundamental importance in many branches of pure and applied science. One of the most intriguing concepts of modern tribology, with exciting practical applications, is the idea of frictionless interface sliding in incommensurate contacts, a phenomenon termed superlubricity. Until very recently, observations of superlubric behavior have been limited to nano- and micro-scale graphitic contacts. One of the major problems in achieving superlubricity using such homogeneous graphitic contacts stems from the fact that graphene tends to spontaneously lock into high-friction states that suppress superlubricity. This fundamental problem has been resolved in our recent studies predicting theoretically and computationally, and thereafter demonstrating experimentally, that *microscale heterogeneous* layered material junctions exhibit robust superlubricity under ambient conditions and room temperature.

In this talk I will discuss results of fully atomistic numerical simulations of static and dynamical properties of graphite/graphite and graphite/hexagonal boron nitride (*h*-BN) junctions. We found that structural superlubricity at interfaces between graphite and *h*-BN persists even for the aligned contacts sustaining external loads. A negative friction coefficient, where friction is reduced upon increasing normal load, was predicted. It was demonstrated that further control over the physical properties of 2D layered materials can be gained via tuning the aspect-ratio of nanoribbons.

Scaling up structural superlubricity towards macroscopic dimensions inevitably involves forming junctions between surfaces of polycrystalline nature. The effects of corrugated grain boundaries on the frictional properties of extended planar graphitic contacts incorporating a polycrystalline surface were investigated via molecular dynamics simulations. This study revealed that collective dynamic effects at polycrystalline graphite grain boundaries may lead to unusual nonmonotonic variation of the friction with normal load and temperature. Our results are expected to be of general nature and should be applicable to other van der Waals heterostructures.

Colloidal AFM probes sliding on graphite: triboinduced material transfer, atomic-scale friction and superlubricity

Renato Buzio[†], Andrea Gerbi[†], Cristina Bernini[†], Luca Repetto[‡], Andrea Vanossi^{†,§}

[†] CNR-SPIN, C.so F.M. Perrone 24, 16152 Genova, Italy

[‡] Dipartimento di Fisica, Università degli Studi di Genova, Via Dodecaneso 33, 16146 Genova, Italy

[†] International School for Advanced Studies (SISSA), Via Bonomea 265, 34136 Trieste, Italy

[§] CNR-IOM Democritos National Simulation Center, Via Bonomea 265, 34136 Trieste, Italy

Colloidal probe Atomic Force Microscopy (AFM) allows to explore sliding states of vanishing friction, i.e. superlubricity, in mesoscopic graphite contacts [1-3]. Superlubricity is known to appear upon formation of a triboinduced transfer layer, originated by material transfer of graphene flakes from the graphitic substrate to the colloidal probe. Previous studies suggest that friction vanishes due to crystalline incommensurability at the newly formed interface [1]. However this picture still lacks several details, such as the roles of the tribolayer roughness and of loading conditions. In this talk we discuss recent colloidal probe AFM experiments addressing the friction response of micrometric beads - of different size and pristine surface roughness - sliding on graphite under ambient conditions [3,4]. We show that such tribosystems undergo a robust transition towards a low-adhesion, low-friction state dominated by localized mechanical interactions at one dominant triboinduced nanocontact. Atomic-scale friction force spectroscopy reveals that such nanocontact can be superlubric or dissipative, in fact undergoing a load-driven transition from dissipative stick-slip to continuous superlubric sliding. This behavior is excellently described by the thermally-activated, single-asperity Prandtl-Tomlinson model. Our results indicate that upon formation of the transfer layer, friction depends on the energy landscape experienced by the topographically-highest triboinduced nanoasperity. Finally, we comment on the friction response of colloidal probes intentionally functionalized by graphene flakes from liquid solutions, and we underline remarkable analogies with the superlubric behavior enabled by the triboinduced nanocontacts. These findings are discussed in light of strategies to achieve robust mesoscale superlubricity.

[1] J. Li, T. Gao, J. Luo, *Superlubricity of graphite induced by multiple transferred graphene nanoflakes*. Adv. Sci. 5 (3), 1700616 (2018)

[2] K. Yu, Y. Peng, H. Lang, S. Ding, Y. Huang, *Material transfer mechanism for fabrication of superlubricity interface by reciprocating rubbing on graphite under high contact stress*, Carbon 188, 420 (2022)

[3] R. Buzio, A. Gerbi, C. Bernini, L. Repetto, A. Vanossi, *Graphite Superlubricity Enabled by Triboinduced Nanocontacts*. Carbon 184, 875 (2021)

[4] R. Buzio, A. Gerbi, C. Bernini, L. Repetto, A. Vanossi, *Colloidal AFM probes sliding on graphite: triboinduced material transfer, atomic-scale friction and superlubricity*, in preparation (2022)

Fluid-electrons interactions in carbon nanomaterials

Alessandro Siria

CNRS and Ecole Normale Supérieure, Paris

Transport of fluid across or at the interface of carbon unveiled unexpected properties in terms of very fast permeation, non-linear ionic transport and sieving and even energy storage and harnessing. These results highlight the subtle interactions of water and charges with the carbon surface. Classically, the interaction of a fluid with a solid wall is based on picturing the solid as a static periodic potential that acts on the fluid molecules: interactions result from collisions on the surface roughness, as flows induced on the roughness scale dissipate mechanical energy. However, recent results for fluid and ion transport in carbon nanotubes and nanochannels made of graphitic materials have pointed out the limits of such standard description for fluid-solid interactions and existing couplings of liquid transport with electronic degrees of freedom inside the confining walls.

In this talk we will firstly recall the first experimental results on ultralow friction of water at the carbon interface; we will then shortly present a unified theory for the electronic effects on the interfacial hydrodynamic friction. Finally we will present recent results on the generation of electric current in a few-layer graphene sample by the displacement of a sub-micrometer scale liquid droplet along its surface. Our results point to a peculiar momentum transfer mechanism between fluid molecules and charge carriers in the carbon walls mediated by phonon excitations in the solid.

Energy dissipation on twisted bilayer graphene at magic angle twist

A. Ollier¹, M. Kisiel¹, U. Gysin¹, E. Tosatti² and E. Meyer¹

¹ *Department of Physics, University of Basel, Klingelbergstrasse 82, 4056-Basel, Switzerland*

² *SISSA, Via Bonomea 265, Trisets 34136, Italy*

Understanding nanoscale energy dissipation is nowadays among few priorities particularly in quantum systems. Whilst traditional Joule dissipation omnipresent in today's electronic devices is well understood, the energy loss of the strongly interacting electron systems remains largely unexplored. Twisted bilayer graphene (tBLG) is a host of interaction-driven correlated insulating phases, when the relative rotation is close to the magic angle (1.08°).

Here, we report on low temperature (5 K) nanomechanical energy dissipation of tBLG measured by sharp tip of the pendulum atomic force microscope (pAFM). Ultrasensitive cantilever tip acting as oscillating plunger gate over the quantum device showed giant dissipation peaks attributed to different fractional filling of the flat energy bands. Dissipation spectroscopy allows to determine the twist angle distribution of tBLG. Thus, nanomechanical energy dissipation provides a rich source of information on the dissipative nature of the correlated electronic system of tBLG, with implications for coupling a mechanical oscillator to the quantum devices. Application of magnetic fields provoked strong oscillations of the force and dissipation signal which is strongly enhanced for fractional $3/4$ band filling.

Nature of dynamic friction in a humid hydrophobic nanocontact

Olivier Noël^{1)*}, Pierre-Emmanuel Mazeran²⁾, and **Igor Stanković**^{3)†}

¹⁾IMMM, UMR CNRS 6283, Le Mans Université,

Av. O. Messiaen, 72085 cedex 09, Le Mans, France

²⁾ Sorbonne universités, Université de Technologie de Compiègne, UMR CNRS 7337, Roberval, Centre de recherche de Royallieu – CS 60319-60203 Compiègne cedex, France

³⁾ Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade, University of Belgrade, 11080 Belgrade, Serbia

*Corresponding authors: * olivier.noel@univ-lemans.fr, † igor.stankovic@ipb.ac.rs

The physics of dynamic friction on water molecule contaminated surfaces is still poorly understood. In line with the growing interest in hydrophobic contact for industrial applications, this paper focuses only on friction mechanisms in such interfaces. As a commonly used material, contact with graphite is considered in a twin-fold approach based on experimental investigations using an atomic force microscopy technique combined with molecular dynamic simulations.

AFM circular mode, used in this study, represents a novel experimental approach that provides a strictly controlled velocity and distance overextended sliding paths, see Fig. 1(a). This mode leads to a relative motion of the contact, without acceleration, deceleration, and any rest periods during sliding which necessarily occur with the conventional back and forth scanning mode. Our results demonstrate that a droplet may form by the accumulation of the adsorbed water (as a packman swallowing smaller water droplets) and stay within the sliding hydrophobic nanocontact, see Fig. 1(b). Then, the nature of the dynamic friction mechanism has been elucidated by considering the resistance of the water droplet driven by one side of the moving contact. We demonstrate that an intuitive paradigm must be refined, which asserts that water molecules are squeezed out of a hydrophobic contact. As a consequence, we introduce a new mechanism considering a droplet produced within the sliding nano-contact by the accumulation of water adsorbed on the substrate. Hence, our findings highlight new routes for controlling water-mediated friction in the air.

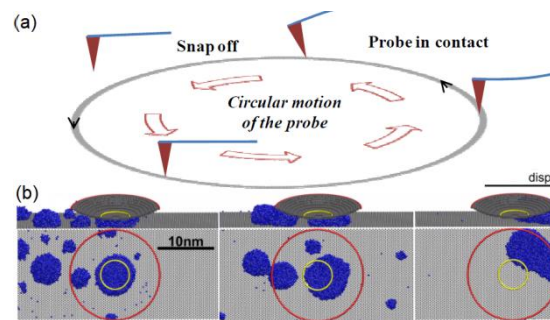


Fig 1. (a) Circular mode coupled with the adhesion force/coefficient of friction spectra. (b) Accumulation of adsorbed water on moving hydrophobic substrate. Distance between successive images is 10nm, $v=1m/s$.

[1] O. Noël, P.-E. Mazeran, I. Stanković, **Nature of dynamic friction in a humid nanocontact, submitted**

Molecular Nanotribology: Nanomanipulation & Dynamics of Single-Molecules at Surfaces.

J.G. Vilhena^{1,2}, Remy Pawlak², Philipp D'Astolfo², Shi-Xia Liu², Silvio Decurtins³, Thilo Glatzel², Alexis Baratoff², Ernst Meyer²

1 – Dep. de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, Madrid

2 - Department of Physics, University of Basel, Klingelbergstrasse 82, Basel, CH 4056

3 - Department of Chemistry and Biochemistry, University of Berne, Freiestrasse 3, Berne, CH 3012

Understanding the motion/dynamics of a single molecule over a surface is a problem of a paramount importance in designing advanced molecular nanostructures/assemblies capable of meeting specific needs[1,2,3]. The interest is better realized by the broad spectrum of promising applications including molecular electronic devices, tribology/corrosion inhibition, and 3D nanopatterning[4]. One possible route to achieve a higher control on molecular diffusion along predetermined pathways would be to access the single-molecule mechanics during their on-surface displacements[5]. This in turn would provide a mean to rationally design molecules with improved assembly/diffusion properties. Nevertheless, to date, understanding the interplay between molecule mechanics, surface displacements and dynamics at a atomic level is highly challenging as it requires knowing not only the forces needed to manipulate them but also to relate them with particular molecular/atomic motion.

Almost 20 years passed after the first scanning probe microscopy[6] atomic-manipulation until it became possible to record the time variations of mechanical forces during manipulation[7]. As this technique[7,8,11,12] – *cryo-force-spectroscopy* – relies on a dynamic AFM operated at 4.8K in Ultra-High-Vacuum it allow us to perform successive manipulations a in a clean and controlled environment but also enable us to characterize both the surface and the molecule with atomic resolution prior and after the manipulation. This breakthrough opened new and exciting possibilities to explore mechanical properties at a single molecule level with an unrepresented resolution and control over the system. In this talk I shall discuss some of the major achievement and the versatility of this technique including: the discovery of a state of almost vanishing friction of graphene nanoribbons when sliding over a gold surface[8,9,10]; measuring the stiffness of a single DNA nucleotide and the detection[11] of a C-C bond twist at a single bond level[12]. Altogether this provides a comprehensive understanding of complex on-surface dynamics of the molecules over surfaces and how dynamic balancing of intra-molecular mechanics and surface comensurability play out in a broad range of conditions.

References:

- [1] Vanossi, A. et al. Rev. Mod. Phys. 85, 529 (2013).
- [2] Manini, N. et al. Adv. Phys. X 2 (3), 569 (2017).
- [3] Moresco, F. et al. Phys. Rev. Lett. 87, 088302 (2001).
- [4] Tao, Feng. Pure Appl. Chem. 80, 45 (2008).
- [5] Kudernac, T. et al. Nature 479, 208–211 (2011).
- [6] Chiaravalloti et al. Nature Mater 6, 30 (2007).
- [7] S Kawai et al. PNAS 111(11), 3968 (2013).
- [8] S Kawai et al. Science 351(6276), 957 (2016).
- [9] Lorenzo Gigli et al. 2D Materials 4, 045003 (2017).
- [10] Lorenzo Gigli et al. Nanoscale just accepted (2019).
- [11] R. Pawlak, J.G. Vilhena et al, Nat. comms 10, 685 (2019).
- [12] J.G. Vilhena, R. Pawlak, et al. Accepted in PRL (2022)

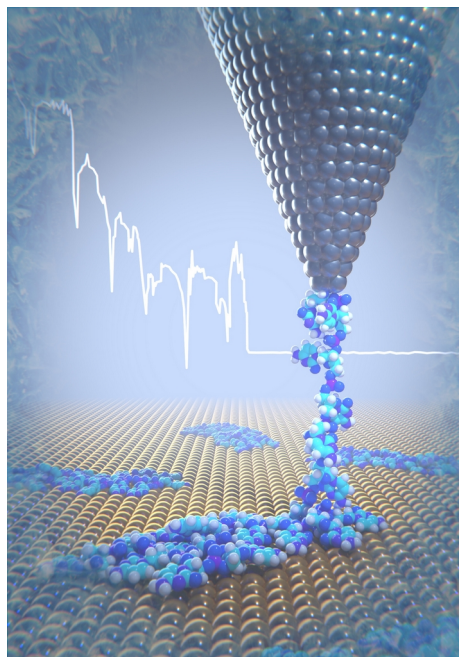


Figure 1: Single molecule cryo-force spectroscopy: Lifting a single-stranded DNA molecule deposited over Au(111).

How adhesion may interfere in friction mechanisms of viscoelastic materials ?

Olivier NOEL¹, Pierre-Emmanuel MAZERAN², Laure FABIE¹, Anh-Dung NGUYEN¹

1. Institut des Molécules et de Matériaux du Mans, UMR 6283, Université du Mans, France

2. Laboratoire Roberval, UMR 7337, Université de Technologie de Compiègne, Compiègne, France

At the nanoscale, the friction forces are known to be strongly dependent on the sliding speed. Typically, for a 'dry' contact, they increase linearly with a logarithmic variation of the sliding speed, in good agreement with the Prandtl-Tomlinson model [1]. On the other hand, for hydrophilic surfaces and in the presence of a capillary meniscus (referred as 'wet' contact), the frictional force decreases linearly with the logarithm of the sliding speed [2]. In the case of polymers, Tocha et al [3] showed that the frictional force passes through a maximum as the sliding speed evolves. This transition in frictional force is legitimately associated with the β -relaxation of polymers (Rotation of $-(CO)OCH_3$ groups in the case of *PMMA*). However, the mechanisms for linking this mechanical transition to the frictional force on these polymer substrates are still very poorly understood. For these materials, contact mechanics models such as *JKR* [4] or *DMT* [5] show that adhesion forces cannot be neglected. In particular, these forces are likely to deform the surfaces in the vicinity of a contact and to generate an adhesive bond. In this talk, I propose an experimental study of the influence of the adhesion force in a sliding nano-contact for the case of polymeric materials. The substrates used are glassy polymers at room temperature, such as poly-methyl methacrylate (*PMMA*) and polycarbonate (*PC*). Experimentally, the study is carried out using an original protocol, the circular *AFM* mode combined with the force spectroscopy mode [6] allowing to measure in a quasi-stationary regime and simultaneously, the adhesion forces and the friction laws for different sliding speeds.

- [1] L. Prandtl, Ein Gedankenmodell zur kinetischen Theorie der festen Körper, *Z. Angew. Math. Mech.* 8, 85–106 (1928) and G. A. Tomlinson, A molecular theory of friction, *Philos. Mag.* 7, 905–939 (1929).
- [2] O.Noel, P-E Mazeran, H.Nasrallah, Sliding velocity dependence of adhesion in a nanometer-sized contact, *Physical Review Letters*, 108, 015503 (2012).
- [3] Tocha et al. [3] *Soft Matter*, 5, 1489, (2009).
- [4] K.L. Johnson, K. Kendall, and A.D. Roberts., « Surface Energy and the Contact of Elastic Solids », *Proc. R. Soc. Lond. Ser. A.*, vol. 324, 1971, p. 301.
- [5] B. V. Derjaguin and V. M. Muller and Y. P. Toporov, Effect of contact deformations on the adhesion of particles, *J. Colloid Interface Sci.* 53 (1975) 314-325.
- [6] H.Nasrallah, P-E Mazeran, O.Noel, Circular mode: A new scanning probe microscopy method for investigating surface properties at a constant and continuous scanning velocities, *Rev. Sci. Instrum.* 82, 113703 (2011).

THERMAL FRICTION ENHANCEMENT IN ZWITTERIONIC MONOLAYERS

Melisa M. Gianetti,¹ Roberto Guerra,¹ Andrea Vanossi,²

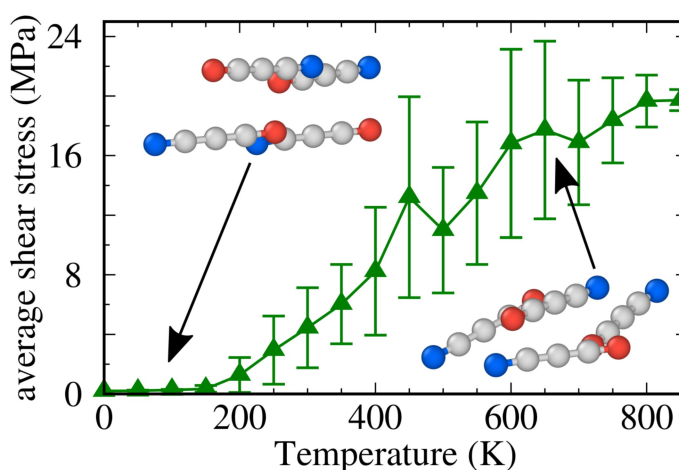
Michael Urbakh,³ and Nicola Manini¹

¹Dip. Fisica, Università degli Studi di Milano, 20133 Milano, Italy

²CNR-IOM & SISSA, 34136 Trieste, Italy

³School of Chemistry, Tel Aviv University, Tel Aviv 6997801, Israel

ABSTRACT: We introduce a model for zwitterionic monolayers and investigate its tribological response to changes in applied load, sliding velocity, and temperature by means of molecular-dynamics simulations. The proposed model exhibits different regimes of motion depending on temperature and sliding velocity. We find a remarkable increase of friction with temperature, which we attribute to the formation and rupture of transient bonds between individual molecules of opposite sliding layers, triggered by the out-of-plane thermal fluctuations of the molecules' orientations. To highlight the effect of the molecular charges, we compare these results with analogous simulations for the charge-free system.



As a further step, we introduce an electric field perpendicular to the sliding direction. This electric field affects the average angular orientation of the dipolar heads of the zwitterionic molecules, resulting in significant changes in friction. Friction initially increases with an electric field up to $\lesssim 5$ GV/m, and it then it decreases beyond this value. An applied load tends to counter the orientating effect of the electric field, leading to a negative friction coefficient.

These findings are expected to be relevant to the nanoscale rheology and tribology of locally-charged lubricated systems such as, e.g., experiments performed on zwitterionic monolayers, phospholipid micelles, or confined polymeric brushes probed in a surface-force apparatus.

Hard particle adhesion and on the stability of spinning asteroids

B.N.J. Persson^{1,2}

¹*PGI-1, FZ Jülich, Germany, EU*

²*www.MultiscaleConsulting.com*

Most asteroids with a diameter larger than ~ 300 m are rubble piles i.e., consisting of more than one solid object. All asteroids are rotating but almost all asteroids larger than ~ 300 m rotate with a period longer than 2.3 hours, which is the critical period where the centrifugal force equals the gravitational force. This indicates that there are nearly no adhesive interaction forces between the asteroid fragments. We show that this is due to the surface roughness of the asteroid particles which reduces the van der Waals interaction between the particles by a factor of 100 for micrometer sized particles and even more for larger particles. We show that surface roughness results in an interaction force which is independent of the size of the particles, in contrast to the linear size dependency expected for particles with smooth surfaces. Thus, two stone fragments of size 100 nm attract each other with the same non-gravitational force as two fragments of size 10 m.

We study the humidity dependency of the adhesion (or pull-off) force between granite fragments and a silica glass plate. The particles bind to the glass plate via capillary bridges. The granite particles are produced by cracking a granite stone in a mortar and have self-affine fractal surface roughness. Theory shows that the surface roughness results in an interaction force between stone fragments and the glass plate which is independent of the size of the particles, in contrast to the linear size dependency expected for particles with smooth surfaces. We measure the adhesion force by depositing the granite particle powder, with particle sizes ranging from mm to μm (or less), on the glass plate. By turning the glass plate upside-down all particles with a gravitational force larger than the adhesion force will fall-off the glass plate. By studying the size (and hence the mass) of biggest still attached particles we obtained the adhesion force, which is found to be in good agreement with the theory prediction.

Effects of friction in active matter

*Hartmut Löwen*¹

¹Heinrich-Heine Universität Düsseldorf, 40225 Düsseldorf, Germany

Active particles which are self-propelled by converting energy into mechanical motion represent an expanding research realm in physics and chemistry. For micron-sized particles moving in a liquid ("microswimmers"), most of the basic features have been described by using the model of overdamped active Brownian motion [1]. Here friction plays the leading role in determining the dynamics. However, for macroscopic particles or microparticles moving in a gas, inertial effects become relevant such that the dynamics is underdamped but friction still plays an important role. Therefore, recently, active particles with inertia have been described by extending the active Brownian motion model to active Langevin dynamics which include inertia [2]. In this talk, recent effects of friction in the field of active matter will be described including: i) the influence of friction on inertial motility-induced phase separation and on the cluster growth exponent [3] and ii) the formation of self-motorized droplet-colloid composites (so-called "droplids").

References

- [1] C. Bechinger, R. di Leonardo, H. Löwen, C. Reichhardt, G. Volpe, G. Volpe, *Reviews of Modern Physics* **88**, 045006 (2016).
- [2] H. Löwen, Inertial effects of self-propelled particles: from active Brownian to active Langevin motion, *Journal of Chemical Physics* **152**, 040901 (2020).
- [3] S. Mandal, B. Liebchen, H. Löwen, *Physical Review Letters* **123**, 228001 (2019).
- [4] J. Grauer, F. Schmidt, J. Pineda, B. Midtvedt, H. Löwen, G. Volpe, B. Liebchen, *Nature Communications* **12**, 6005 (2021).

Rise and growth of critical instabilities in systems under shear

Roberto Guerra

¹Department of Physics, University of Milan, via Celoria 16, 20133 Milan, Italy

Keywords: friction, instabilities, silica, Hessian methods.

Abstract. The dynamics of amorphous matter with frictional interactions cannot be derived in general from a Hamiltonian and therefore displays oscillatory instabilities stemming from the onset of complex eigenvalues in the stability matrix. Here we derive and demonstrate the presence of oscillatory instabilities in a three-dimensional granular packing. We study binary assemblies of spheres of two sizes interacting via classical Hertz and Mindlin force laws for the longitudinal and tangent interactions, respectively. We formulate analytically the stability matrix in three dimensions and observe that a couple of complex eigenvalues emerge at the onset of the instability as in the case of frictional disks in two dimensions. The dynamics then shows oscillatory exponential growth in the mean-square displacement, followed by a catastrophic event in which macroscopic portions of mechanical stress and energy are lost. The generality of these results for any choice of forces that break the symplectic Hamiltonian symmetry is discussed [1].

Furthermore, we study atomic-scale plastic instabilities in a three-dimensional molecular dynamics model of silica glass under quasistatic shear. We identify two distinct types of elementary plastic events, one is a standard quasilocalized atomic rearrangement while the second is a bond-breaking event that is absent in simplified models of fragile glass formers. Our results show that both plastic events can be predicted by a drop of the lowest nonzero eigenvalue of the Hessian matrix that vanishes at a critical strain. Remarkably, we find very high correlation between the associated eigenvectors and the nonaffine displacement fields accompanying the bond-breaking event, predicting the locus of structural failure. Both eigenvectors and nonaffine displacement fields display an Eshelby-like quadrupolar structure for both failure modes, rearrangement, and bond breaking. Our results thus clarify the nature of atomic-scale plastic instabilities in silica glasses, providing useful information for the development of mesoscale models of amorphous plasticity [2].

[1] S. Bonfanti, J. Chatteraj, R. Guerra, I. Procaccia, S. Zapperi, Phys. Rev. E 101, 052902 (2020)

[2] S. Bonfanti, R. Guerra, C. Mondal, I. Procaccia, S. Zapperi, Phys. Rev. E 100, 060602(R) (2019)

PLASTICITY IN NANOSCALE FRICTION: STATIC AND DYNAMIC

John B.Pethica, Trinity College Dublin, Ireland

Owen Brazil, Texas A&M University, TX77840, USA
George M. Pharr, Texas A&M University, TX77840, USA

In classical macroscopic friction bulk plasticity has an important role, but in many investigations of nanoscale single asperity sliding it is absent, with purely interface slip the dominant factor. The connection between nanoscale studies and macroscopic friction systems can thus sometimes be problematic. Explaining the phenomenon of static friction is also difficult. Many industrial applications are more concerned with reducing wear rather than friction and the two are not simply related. Third body particles, irregular surface geometries and compositions, and their effect on lubricant behaviour are important.

This talk will describe the use of a new 2-D nanoindentation system to investigate the initial stages of lateral deformation of contacts¹. The apparatus accesses a much wider range of contact stiffnesses than techniques such as AFM and SFA and can thus study both purely elastic, and plastic deformations.

We show that static friction depends on indent sink-in arising from the combination of lateral and normal stresses. Material yield strain affects the evolution of contact area. As lateral strain increases the limit of junction growth is reached, and the onset of full sliding is controlled by interface friction and tip geometry, broadly in agreement with classical models. If sufficiently small normal loads and smooth tips are used the purely interface sliding and largely wear-free friction seen in AFM and SFA can be observed. Yield strain, tip geometry and interface strength can distinguish the pathways of initial sliding and transition between modes of behaviour. It might also be applied to multi-asperity contacts and friction of rough surfaces.

In these experiments it is shown that the dominant energy dissipation mechanism, as soon as there is steady sliding, is interface slip rather than bulk plastic flow. We comment on the significance for classical models of friction and wear. The mechanisms of frictional energy dissipation and the distinction between constitutive and local atomistic models will be discussed.

1. Brazil, O., Pethica, J.B. & Pharr, G.M., *Proc. R. Soc. A* (2021)0502.
<https://doi.org/10.1098/rspa.2021.0502>

Phase-Transitions in Nano-Friction

Dirk Dietzel and Andrè Schirmeisen

Institute of Applied Physics, Justus-Liebig-Universität Gießen, Gießen, Germany

In current nanotribology, one of the most intriguing questions concerns the atomic scale mechanisms of energy dissipation during the sliding process. Different energy dissipation channels have been proposed, including phonon and electron systems, plastic deformation, and crack formation. Still, how energy is coupled into these channels is debated, even for clean, low-wear sliding-contacts.

To address such questions, the analysis of phase-transition materials offers a unique approach, since limited but well-defined transformations can be induced if a specific control parameter, for instance the temperature, changes. Varying friction between a slider and the sample can then either be linked to the properties of different phases or the phase transition itself, with potentially a direct coupling to the reorganization of the material.

The potential of analyzing phase transitions in nano-friction is demonstrated for different examples. By analyzing a superconducting phase transition of BSCCO using friction force microscopy, the continuously decreasing friction in the superconducting state can be correlated to the number of remaining normal state electrons [1]. In addition, a structural transition of the charge density wave material 1T-TaS₂ is linked to a process where the AFM-tip gradually induces local transformations of the material close to the spinodal point [2]. Based on load and velocity dependent friction analysis this excitation process can be described as a thermally activated and shear assisted process with a decreasing energy barrier close to the phase transition. Finally, we find that superlubric Sb nanoparticles sliding on HOPG reach different levels of friction when switching from amorphous to the crystalline state. These experimental findings offer unique views into the atomic mechanisms of nano-friction, and in particular show how phase transitions influence the dominating energy dissipation channels.

[1] W. Wang, D. Dietzel, and A. Schirmeisen, *Science Advances* 6, eaay0165 (2020).

[2] E. Panizon, T. Marx, D. Dietzel, F. Pellegrini, G. Santoro, A. Schirmeisen, and E. Tosatti, *New Journal of Physics* 20, 023033 (2018).

Anisotropic Frictional Response of Suspended Graphene

Andrea Mescola¹, Andrea Silva^{2,3}, Ali Khosravi², Andrea Vanossi^{2,3}, Erio Tosatti^{2,3,4}, Sergio Valeri^{1,5} and Guido Paolicelli¹

1. CNR-Istituto Nanoscienze - Centro S3, Via Campi 213, 41125 Modena, Italy.
2. CNR-IOM, Consiglio Nazionale delle Ricerche - Istituto Officina dei Materiali, c/o SISSA, 34136, Trieste, Italy
3. International School for Advanced Studies (SISSA), 34136 Trieste, Italy
4. International Centre for Theoretical Physics ICTP, 34151 Trieste, Italy
5. Department of Physics, Informatics and Mathematics, University of Modena and Reggio Emilia, Via Campi 213 41125 Modena, Italy.

Abstract

The rheological behavior of graphene and other 2D materials' is currently investigated under different conditions ranging from sheets deposited on specific substrates to totally suspended films, both free and strained. While for supported graphene the role of the underlying substrates has been found to be pivotal in tuning the strain and, consequently, its frictional response¹, less is known about the rheological behavior of suspended membranes, specifically in presence of anisotropic constraints at the boundaries. Indeed, the layered systems investigated so far are generally isotropically suspended, i.e. clamped on a circular hole²⁻⁴. On the contrary, here we study the AFM friction response of single layer CVD (Chemical Vapor Deposition) graphene totally suspended on an asymmetric geometry of long narrow grooves⁵. The frictional dissipation during sliding as measured by AFM and analysed with friction-vs-load curves, reveals an anisotropic character: i.e., higher COF (Coefficient Of Friction) when sliding parallel to the groove axis, and systematically lower along the orthogonal direction. The absence of a velocity dependence in the recorded data suggests, in both directions, the occurrence of a stick-slip dynamical regime and the deformation induced by the sliding probe itself, which represents the most straightforward case of strain induction⁶, seems to be particularly relevant in this system. Complementary molecular dynamics (MD) simulations specifically mimicking the peculiar suspended clamping geometry, reveal indeed an anisotropic mechanical deformation of the graphene membrane induced by the loading action of the tip, revealing a distinct effective softness of the contact along the two directions. The outcome of the friction-vs-load curves from this computational approach perfectly matches the experimental results, indicating higher COF when sliding parallel to the groove axis.

References

1. Mescola, A. *et al.* Graphene Confers Ultralow Friction on Nanogear Cogs. *Small* **17**, 2104487 (2021).
2. Deng, Z. *et al.* Nanoscale Interfacial Friction and Adhesion on Supported versus Suspended Monolayer and Multilayer Graphene. *Langmuir* **29**, 235–243 (2013).
3. Kitt, A. L. *et al.* How Graphene Slides: Measurement and Theory of Strain-Dependent Frictional Forces between Graphene and SiO₂. *Nano Lett.* **13**, 2605–2610 (2013).
4. Zhang, S. *et al.* Tuning friction to a superlubric state via in-plane straining. *Proc Natl Acad Sci USA* **116**, 24452–24456 (2019).
5. Mescola, A., *et al.* Anisotropic Rheology of Suspended Graphene. (*in preparation*) (2022).
6. Lee, C., Wei, X., Kysar, J. W., Hone, J. & Marrow, J. Measurement of the Elastic Properties and Intrinsic Strength of Monolayer Graphene. *Science* **321**, 382–385 (2008).

Atomistic Mechanisms of Friction for MoS₂ and Beyond

Ashlie Martini, University of California Merced

Molybdenum disulfide is a lamellar solid used to lower friction and wear in applications ranging from additives in specialty greases to coatings on components that operate in space. However, the tribological behavior of MoS₂ is extremely sensitive to synthesis parameters, the environment, and operating conditions, which impedes accurate and consistent prediction of performance in lubricant or component design. One approach to understanding this very complex behavior is to break it down into a fundamental “unit” of tribology, i.e., sliding of a single asperity. Single asperity friction is studied using atomic force microscopy and matched molecular dynamics simulations. Here, we share examples of such studies of the atomistic origins of temperature, velocity, and orientation dependence of friction, as well as head-to-head comparisons between MoS₂ and other 2D materials, including graphene, a graphene-MoS₂ heterostructure, and other transition metal dichalcogenides. These studies suggest correlations between friction behavior at the single asperity scale and fundamental atomic features of the materials that can ultimately be the starting point to guide design with MoS₂ and beyond.

NON-EQUILIBRIUM DYNAMICS AND NANOFRICTION IN ION COULOMB CRYSTALS

Lars Timm¹, Jan Kiethe², Hendrik Weimer¹, Luis Santos¹, and Tanja E. Mehlstäubler^{1,2}

¹Leibniz Universität Hannover, 30167 Hannover, Germany

²PTB, 38116 Braunschweig, Germany

Single trapped and laser-cooled ions in Paul traps allow for a high degree of control of atomic quantum systems. They are the basis for modern atomic clocks, quantum computers and quantum simulators. Our research aims to use ion Coulomb crystals, i.e. many-body systems with complex dynamics, for precision spectroscopy. This paves the way to novel optical frequency standards for applications such as relativistic geodesy and quantum simulators in which complex dynamics becomes accessible with atomic resolution.

The high-level of control of self-organized Coulomb crystals open up a fascinating insight into the non-equilibrium dynamics of coupled many-body systems, displaying atomic friction and symmetry-breaking phase transitions. We discuss the creation of topological defects in 2D crystals and present recent results on the study of tribology and transport mediated by the topological defect, discussing both classical and quantum regimes.

- [1] J. Kiethe *et al.*, Nat. Commun. **8** (2017) 15364.
- [2] J. Kiethe *et al.*, New J. Phys. **20** (2018) 123017.
- [3] L. Timm, *et al.*, Phys. Rev. Research 2, 033198 (2020)
- [4] L. Timm, *et al.*, Phys. Rev. Research 3, 043141, (2021)

Markov dynamics and entropy production in a Prandtl–Tomlinson model

Alberto Petri

CNR - Istituto dei Sistemi Complessi, Dipartimento di Fisica
Università Sapienza, Rome, Italy

The so called Prandtl–Tomlinson model represents the dissipative motion of a particle on a periodic substrate and has recently seen renewed interest for its suitability to describe atomic force microscopy. We consider the model in the case of a constant driving force and in the presence of thermal fluctuations and show that its dynamics can be effectively reproduced by a simplified description obtained through a Markov process, even in the presence of potentials with several minima. From a general point of view, systems description in terms of Markov chains can be of help to make quantitative connection with experiments, and as a guide to formulate more detailed models, especially when dealing with complicated potentials. In the case considered here, besides obtaining the average velocity and friction at varying driving force and temperature, we take advantage of this approach calculating the entropy produced by the system. In the case of a potential with a single minimum we derive an explicit relation of the entropy production rate with the external force and the mobility at low temperatures, and find that the coefficient relating the entropy production to the force is a non monotonic function of the temperature.

- D. Lucente, A. Petri and A. Vulpiani, *Physica A* 572, 125899 (2021)

Title:

Collective colloidal dynamics on ordered and disordered landscapes

Authors:

Ralph Stoop¹, Arthur Straube¹, Philipp Maass² and Pietro Tierno^{1,3,4}

¹ Departament de Física de la Matèria Condensada, Universitat de Barcelona, 08028, Barcelona, Spain

² Universität Osnabrück, Fachbereich Physik, Barbarastrasse 7, D-49076 Osnabrück, Germany.

³ Universitat de Barcelona Institute of Complex Systems (UBICS), Spain.

⁴ Institut de Nanociència i Nanotecnologia, Universitat de Barcelona, Barcelona, Spain.

Abstract:

In this talk, I will discuss recent results obtained in my group by using paramagnetic colloidal particles driven across two dimensional periodic and random magnetic landscapes. These landscapes are generated by thin ferromagnetic films that provide an array of cylindrical ferromagnetic domains, also named “magnetic bubbles”. An external rotating magnetic field can modulate the periodic energy landscape and induce a directed particle transport via a travelling wave like mechanism [1,2]. In the first part of the talk, I will show that when the particles are forced to cross a direction that intersects two crystallographic axes of the lattice, collective effects induce transversal current and directional locking at high density via a spontaneous symmetry breaking [3,4]. In the second part of the talk, I will explore the case of disordered systems and the corresponding current density relationship. I will explain two novel effects. The first one originates from particle sizes nearly commensurate with the substrate in combination with attractive pair interactions that we explain by an exactly solvable model of constrained cluster dynamics. It governs the colloidal flow at small densities and leads to a superlinear current increase. The second effect is a defect-induced breakup of coherent cluster motion, leading to an effective jamming of particle flow at higher densities. Finally, I will show that a lattice gas model with a parallel update is able to capture the experimental findings of this complex many-body system [5].

References:

1. P. Tierno, T. H. Johansen, T. M. Fischer Phys. Rev. Lett. 99, 038303 (2007).
2. P. Tierno, T. M. Fischer, Phys. Rev. Lett. 112, 048302 (2014).
3. C. Reichhardt, C. J. Olson Reichhardt, Phys. Rev. Lett. 100, 167002 (2008).
4. R. L. Stoop, A. V. Straube, T. H. Johansen, P. Tierno, Phys. Rev. Lett. 124, 058002 (2020).
5. D. Lips, R. L. Stoop, P. Maass, P. Tierno, Comm. Phys. 4, 224 (2021).

Understanding the Rheology of Nanocontacts

Ali Khosravi^{1,2,3}, Antoine Lainé⁴, Andrea Vanossi³, Jin Wang¹, Alessandro Siria⁴, and Erio Tosatti^{1,2,3}

¹*International School for Advanced Studies (SISSA), I-34136 Trieste, Italy*

²*International Centre for Theoretical Physics, I-34151 Trieste, Italy*

³*CNR-IOM, Consiglio Nazionale delle Ricerche - Istituto Officina dei Materiali, c/o SISSA, 34136, Trieste, Italy*

⁴*Laboratoire de Physique de l'École Normale Supérieure, ENS, Université PSL, CNRS, Sorbonne Université Université Paris-Diderot, Sorbonne Paris Cité, UMR CNRS 8550, Paris, France*

Mechanical stiffness, as opposed to softness, is a fundamental property of solids. Its persistence or rheological evolution in vibrating solid-solid nanocontacts is important in physics, materials science and technology. A puzzling apparent liquefaction under oscillatory strain, totally unexpected at room temperature, was suggested by recent experiments on solid gold nano-junctions. Here we show theoretically that realistically simulated nanocontacts actually remain crystalline even under large oscillatory strains. Tensile and compressive slips, respectively of “necking” and “bellying” types, do take place, but recover reversibly even during fast oscillatory cycles. We also show that, counterintuitively, the residual stress remains tensile after both slips, driving the averaged stiffness from positive to negative, thus superficially mimicking a liquid’s. Unlike a liquid, however, rheological softening occurs by stick-slip, predicting largely frequency independent stiffness with violent noise in stress and conductance, properties compatible with experiments. The baffling large amplitude rheology of gold nanocontacts and its consequences should apply, with different parameters, to many other metals.

Dissipation and lubrication of solid-liquid nanointerfaces: complex balance of substrate topography, molecular diffusion and environmental conditions

Clodomiro Cafolla

Department of Physics, Durham University, DH1 3LE, UK

The dynamical and lubricating properties of solid-liquid nanointerfaces control many natural and industrial processes, from the functioning of our joints, to water purification and engine efficiency. Still, our understanding is largely based on semi-empirical macroscopic models, with only a few direct links between molecular-level effects and the technologically relevant macroscopic forces¹⁻³. Furthermore, experimental and computational methods tend to assume an ideal solid-liquid interface, whereas in real life scenarios singularities and environmental factors significantly modify the system behaviour.

Here, we address the problem by Atomic Force Microscopy (AFM), complemented by molecular dynamics simulations, to build a functional picture of two model lubricated systems down from single molecule details and up to molecular group effects (~100 nm).

First, using polar model lubricants, we show the molecular mechanisms behind the detrimental impact of surface singularities and humidity on their lubricating properties¹⁻². Defects promote the ordering of fluid molecules, with the elastic-like characteristics of the boundary layer being responsible for an increase in lubricated friction¹. The fluid effective dynamic response is detrimentally affected by the combined effect of temperature and humidity with water nanodroplets, adsorbed to metal surfaces from ambient humidity, appearing through a thermally-nucleated process, modifying the surface wetting properties and creating local pinning points².

In the case of non-polar model fluids, the results suggest that the hydrogen bond network of the interfacial water induces a glassy-like behaviour that dominates lubrication and molecular diffusion. Here, epitaxial effects and the surface charge density directly influence the mobility of the water molecules and indirectly modulate the density of the hydration layers. Adding salt to the system promotes the spatial ordering of the water molecules into mesoscale domains further away from the surface. The results offer a complementary framework to interpret AFM spectroscopy with soft cantilevers: the AFM tip can probe not only the water densification in the hydration layers, but the dynamic mobility of water molecules and hydrated ions near the interface.

Overall, the results contribute to bridging the current gap between atomistic models and observed macroscale phenomena with the ultimate goal of developing efficient tribological solutions for real-life systems.

1. Cafolla et al., *Science Advances* 6: eaaz3673, 2020
2. Cafolla et al., *Nanoscale* 12: 14504-14513, 2020
3. Cafolla et al. *Scientific Reports* 11: 1-9, 2021

Energy storage and dissipation by forced wetting and drying of nanoporous materials

Alberto Giacomello

Dipartimento di Ingegneria Meccanica e Aerospaziale, Sapienza Università di Roma, Via Eudossiana 18, 00184 Roma, Italy

Heterogeneous lyophobic systems (HLS) are composed of a nanoporous material immersed in a non-wetting liquid – in many cases water. By leveraging the peculiar behavior of nanoconfined liquids, it is possible to design such systems either for storing or for dissipating energy [1]. The simplicity, compactness, and low cost of such systems makes them ideal candidates for a number of applications, including the automotive and aerospace industries.

Dissipation of energy in HLS occurs because the liquid intrusion in nanopores (wetting) occurs, in the general case, at conditions different from those of the extrusion from nanopores (drying). For instance, in the case of pressure cycles, hysteresis between the intrusion and extrusion pressures leads to dissipate a portion of the supplied mechanical energy. On the other hand, materials with low pressure hysteresis can store mechanical energy in the form of interfacial energy and released upon decreasing pressure. The mechanism and the kinetics of wetting and drying both sensitively depend on the level of hydrophobicity, on the geometry, and on the size of confinement [2]. Understanding in detail these wetting and drying phenomena is therefore key to design HLS for a specific application.

In this study, we explore by means of experiments, theory, and molecular dynamics the effect of pore connectivity [3] and elasticity [4] on the intrusion and extrusion of liquids from hydrophobic nanopores. High-pressure water intrusion and extrusion experiments performed on two porous materials with similar nominal diameter and hydrophobicity showed similar behavior for intrusion but qualitatively different ones for extrusion [3]: the first material with cylindrical, independent pores displayed irreversible liquid intrusion, while the second one, characterized by interconnected pores, exhibited extrusion (vapor nucleation) at pressures as large as few megapascals. Leveraging macroscopic capillary models and extensive molecular dynamics simulations we propose an explanation of this peculiar behavior based on the internal morphology of the pores and, in particular, on the presence of small-scale roughness or pore interconnections in the second materials. Additional experiments with mercury confirmed that this mechanism is generic for nonwetting liquids and is indeed connected to the pore topology. The relevance of elasticity in determining liquid extrusion from nanopores will be further analysed [4]. Altogether the present results suggest a rational way to design heterogeneous systems for energy storage or dissipation in which the intrusion and extrusion behavior can be controlled via the pore morphology and elasticity.

References

- [1] V. Eroshenko, R.-C. Regis, M. Soulard and J. Patarin, *J. Am. Chem. Soc.*, 2001, **123**, 8129–8130.
- [2] L. Guillemot, T. Biben, A. Galarneau, G. Vigier and É. Charlaix, *Proc. Natl. Acad. Sci. USA*, 2012, **109**, 19557–19562.
- [3] M. Amabili, Y. Grosu, A. Giacomello, S. Meloni, A. Zaki, F. Bonilla, A. Faik, and C.M. Casciola, *ACS Nano* **2019**, *13*(2), 1728.
- [4] M. Tortora, P. Zajdel, A.R. Lowe, et al. *Nano Letters* **2021**, *21*(7), 2848-2853.

Microscopic mechanisms of frictional aging

Wengen Ouyang^{1*}, Michael Urbakh^{2*}

¹*Department of Engineering Mechanics, School of Civil Engineering, Wuhan University, Wuhan, Hubei 430072, China*

²*Department of Physical Chemistry, School of Chemistry, The Raymond and Beverly Sackler Faculty of Exact Sciences and The Sackler Center for Computational Molecular and Materials Science, Tel Aviv University, Tel Aviv 6997801, Israel.*

ABSTRACT

Frictional aging is observed at a wide range of length- and time-scales, and plays a crucial role in functioning of micro- and nanomachines, as well as in the nucleation and recurrence of earthquakes. Recently, we developed an analytical model for description of frictional aging mediated by dynamical formation and rupture of microscopic interfacial contacts. The model accounts for the presence of various types of contacts at the frictional interface and exhibits three different aging regimes: (i) linear aging at short hold times, (ii) logarithmic (or logarithmic-like) aging for intermediate time scales and (iii) levelling off in the static friction for long hold times. It is demonstrated that the linear aging regime is a universal feature of frictional aging for the interfaces including various types of contacts, and the slope of variation of the static friction with the hold time depends on a distribution of energy barriers for contact formation. The conditions for the existence of a pronounced logarithmic aging regime, covering a long-time interval, have been established. Frictional aging has been found to manifest itself not only in slide-hold-slide measurements, but also in sliding experiments exhibiting stick-slip mode of motion, and a relationship has been established between these two regimes of aging. The predicted dependencies of frictional aging on the normal load and temperature are in good agreement with the experimental observations. Our work shows that experimental studies of load and temperature dependencies of aging, carried out over a wide range of time scales, offer promising opportunities for understanding the microscopic mechanisms of frictional aging and revealing the physical meaning of state variables that determine temporal evolution of friction described by phenomenological rate and state laws.

Unravelling superlubricity and interfacial electrical contact mechanism at single-asperity level

Tianbao Ma

State Key Laboratory of Tribology, Tsinghua University, Beijing 100084, China.

Atomic force microscopy (AFM) has become important tool to understand interfacial phenomenon at single-asperity level. I'll introduce some of our recent works in the searching for superlubricity mechanism of diamond-like carbon (DLC) and electrical contact mechanism across two-dimensional (2D) material interface. (1) DLC has demonstrated macroscale superlubricity experimentally in recent decades. However, the microscopic mechanism still remains unresolved. By precisely controlling the test environment to ultra-high vacuum, superlubricity was achieved by AFM after a two-stage running-in behavior. The friction evolution mechanism has been attributed to ordering structural transformation and transfer film formation [1]. (2) In another work by conductive AFM, we find an atomic modulation of vertical conductance due to the interfacial stacking geometry. Based on the experimental observation, we establish an atomic-scale contact quality model, which provides a direct correlation between the contact conductance and the interfacial atomic geometries [2,3].

References:

- [1] Wang K, et al. Unraveling the Friction Evolution Mechanism of Diamond-Like Carbon Film during Nanoscale Running-In Process toward Superlubricity. *Small*, 2021, 17, 1, 2005607.
- [2] Song A, et al. Fluctuation of interfacial electronic properties induces friction tuning under electric field. *Nano Letters* 2022, 22, 5, 1889-1896.
- [3] Song A, et al. Modelling atomic-scale electrical contact quality across two-dimensional interfaces. *Nano Letters* 2019, 19, 6, 3654-3662.

Moiré-pattern evolution couples rotational and translational friction at crystalline interfaces

Xin Cao^{1,a}, Andrea Silva^{2,3,a}, Emanuele Panizon⁴, Andrea Vanossi^{2,3}, Nicola Manini⁵, Erio Tosatti^{2,4,3}, Clemens Bechinger^{1*}

1 Fachbereich Physik, Universität Konstanz, 78464 Konstanz, Germany

2 CNR-IOM, Consiglio Nazionale delle Ricerche - Istituto Officina dei Materiali, c/o SISSA, Via Bonomea 265, 34136, Trieste, Italy

3. International School for Advanced Studies (SISSA), Via Bonomea 265, 34136 Trieste, Italy

4 The Abdus Salam International Centre for Theoretical Physics (ICTP), Strada Costiera 11, 34151 Trieste, Italy

5 Dipartimento di Fisica, Università degli Studi di Milano, Via Celoria 16, 20133 Milano, Italy

XC and AS contributed equally

The sliding motion of objects is typically governed by their friction with the underlying surface. Compared to friction related to translation, however, rotational friction has received much less attention. Here, we experimentally and theoretically study the rotational depinning and orientational dynamics of two-dimensional colloidal crystalline clusters on periodically corrugated surfaces in the presence of magnetically exerted torques. We demonstrate that the traversing of locally commensurate areas of the moiré pattern through the edges of clusters, which is hindered by potential barriers during cluster rotation, eventually controls its rotational depinning. The experimentally measured depinning thresholds as a function of cluster size strikingly collapse onto a universal theoretical curve which predicts the possibility of a superlow-static-torque state for large clusters. We further reveal a cluster-size-independent rotation-translation depinning transition when lattice-matched clusters are driven jointly by a force and a torque. Our work provides guidelines to the design of nanomechanical devices that involve rotational motions on atomic surfaces.

Open issues in pharmaceutical powders mechanics

Andrea Benassi

Chiesi Pharmaceuticals, Parma (Italy)

While designing pharmaceutical products, and the related manufacturing processes, meso-scale tribology and dissipation problems are often encountered. The flow of powders and other granular media is governed by adhesion and friction at the particle-particle contact points. Confined powders under shear stress sometimes display a stick-slip dynamics. Powder compaction and powder milling are examples of industrial unit operations whose outcome is governed by microscopic plasticity and brittleness properties of single powder particles and grains. Powders and aerosol particles subject to strong shearing conditions can undergo tribo-electrification, generating electrostatic phenomena altering the performances of products and plants. An overview on our recent experimental investigation of these kind of phenomena will be presented. The current limitations preventing both simple models and simulations from being predictive of such phenomena, will be also discussed.

Oscillatory motion of viscoelastic polymer drops on slippery lubricated surfaces

P. Sartori¹, D. Ferraro¹, M. Dassi¹, A. Meggiolaro¹, D. Filippi¹,
A. Zaltron¹, G. Mistura¹, M. Pierno¹

¹*Dipartimento di Fisica e Astronomia “G. Galilei”,
Università di Padova, via Marzolo 8, 35131 Padova (Italy)*

The motion of a drop on a solid surface attracts a lot of attention for its implications on microfluidics and wetting [1]. On a tilted surface, this motion is the result of a balance between the down-plane component of the drop weight and the viscous resistance, plus a capillary force related to the nonuniformity of the contact angle along the drop perimeter [2]. On Slippery Lubricated Surfaces (LIS) a suitable low surface tension lubricating liquid is trapped inside a surface texture [3]. This allows drops of an immiscible fluid to float on the lubricant layer with low friction, even for highly viscous solutions which otherwise would hardly move on solid surfaces [4].

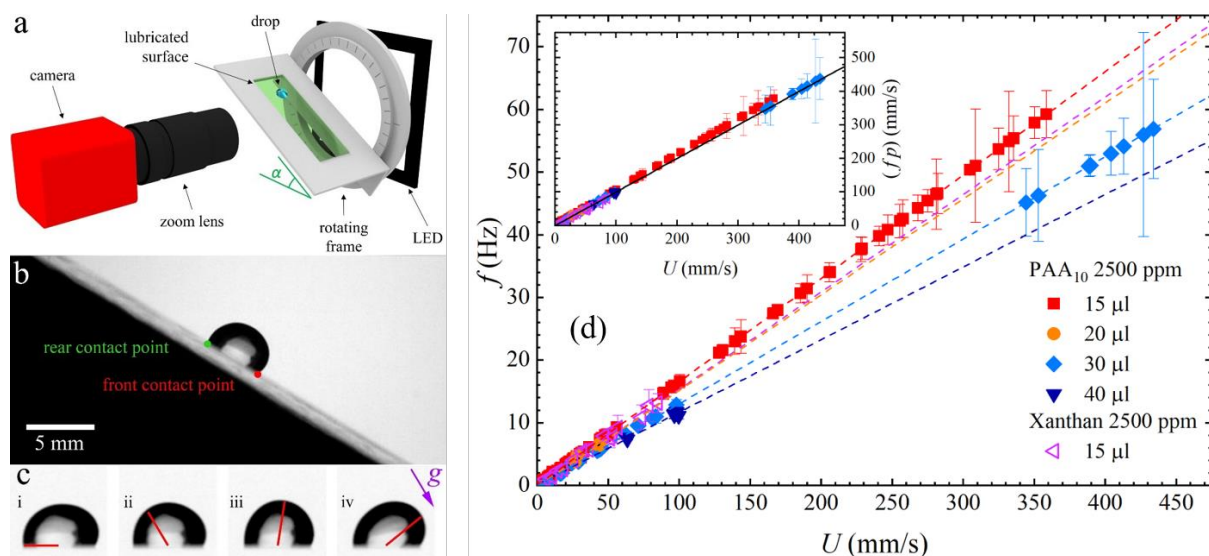
Here we show the gravity induced motion of small viscoelastic drops deposited on inclined lubricated surfaces (Fig.1-a,b). Viscoelastic fluids made of Polyacrylamide (PAA) and Xanthan gum exhibit shear thinning and, more importantly, a significant first normal stress difference N_1 . Despite the homogeneity of the surface and of the fluids, drops of sufficiently high N_1 move down with an oscillating instantaneous speed whose frequency is found to be directly proportional to the average speed and inversely to the drop volume, collapsing on a master curve if the drop boundary is accounted (Fig.1-d). The oscillatory motion is triggered by the polymer rheology, causing the formation of a bulge at the drop rear that starts a rolling motion (Fig.1-c).

[1] G. Mistura, and M. Pierno, *Adv.Phys. X* **2**, 591 (2017).

[2] P.G. De Gennes, F. Brochard-Wyart. and D. Quéré, *Capillarity and Wetting Phenomena: Drops, Bubbles, Pearls, Waves*. (Springer, 2004).

[3] T. S. Wong, S. H. Kang, S. K. Tang, E. J. Smythe, B. D. Hatton, A. Grinthal, and J. Aizenberg, *Nature* **477**, 443 (2011).

[4] S. Varagnolo, D. Filippi, G. Mistura, M. Sbragaglia, and M. Pierno, *Soft Matter* **13**, 3116 (2017)



The nerve pulse as an electromechanical soliton, and how it is related to fluctuations and relaxation timescales in biological membranes

Thomas Heimburg

Niels Bohr Institute, University of Copenhagen, Blegdamsvej 17, 2100 Copenhagen Ø, Denmark

Nerve pulses are usually considered as electrical phenomena. However, measurements show that they also display mechanical changes and reversible variations in temperature. For this reason, we have proposed that the nerve pulse consists of an electromechanical soliton. Biological membranes display a melting transition slightly below body temperature, in which the order of the membrane lipids changes. During this transition, the heat capacity reaches a maximum, as do the volume and area compressibility as well as the relaxation time scales. This results in a frequency-dependent minimum of the sound velocity in the nerve membrane. This fact allows for the generation of solitons that display a remarkable similarity to nerve pulses. We show here how to obtain all relevant information from heat capacity profiles. Further, we show that the relaxation time scales also determine the width of the pulse such that the whole description is self-contained and free of parameters beyond those that can be directly obtained from experiment.

Where did that charge come from?

Karl Olson, Christopher Mizzi, Alex Lin and Laurence Marks

Department of Materials Science, Northwestern University

Almost as old as tribology, triboelectricity dates back to the work of Thales of Miletus in the sixth century BCE. It is demonstrated in high schools, can be a major issue in the processing of pharmaceutical powders, and is key to lightning and even the formation of planets – it is pervasive.

Triboelectricity and tribology shares the same grammatical root “tribo” for friction, and it has been known empirically for centuries that there is a connection. Despite decades of effort, some of which included full incorporation of established tribological processes such as asperity contacts, why charge transfer should occur has baffled scientists. The problem has been that none of the conventional approaches such as differences in work functions or piezoelectricity can explain experiments. There are many less rigorous, somewhat ad-hoc models without basis in other known physics – but these only work in a few cases, and in general fail.

What are we missing?

We have recently pointed out [1] that there is one electromechanical term which had been missed in the analysis: flexoelectricity -- see [2-5]. This is the coupling of strain gradients with polarization, different from piezoelectricity which is strain and polarization. Because it is a gradient term, it becomes very important at the nanoscale and there is now extensive experimental and theoretical evidence that it often dominates.

Asperities are often at the nanoscale, and deform during contact. It turns out that the polarization, and consequently the potential differences that the asperity deformations lead to can be several volts or even much more, certainly large enough to drive charge transfer [1]. This talk will discuss some of the analysis for a range of materials and geometries [6], plus work on the flexoelectric band-bending of sliding Schottky contacts based upon both experimental and theoretical data [7].

1. Mizzi, C.A., A.Y.W. Lin, and L.D. Marks, *Does Flexoelectricity Drive Triboelectricity?* Phys Rev Lett, 2019. **123**(11): p. 116103 <https://doi.org/10.1103/PhysRevLett.123.116103>.
2. Bursian, E.V. and O.I. Zaikovskii, *Changes in the curvature of a ferroelectric film due to polarization*. Soviet Physics - Solid State, 1968. **10**(5): p. 1121-1124.
3. Hong, J.W. and D. Vanderbilt, *First-principles theory of frozen-ion flexoelectricity*. Physical Review B, 2011. **84**(18): p. 5 <https://doi.org/10.1103/PhysRevB.84.180101>.
4. Zubko, P., G. Catalan, and A.K. Tagantsev, *Flexoelectric Effect in Solids*, in *Annual Review of Materials Research, Vol 43*, D.R. Clarke, Editor. 2013, Annual Reviews: California. p. 387-421. <https://doi.org/10.1146/annurev-matsci-071312-121634>
5. Stengel, M., *Unified ab initio formulation of flexoelectricity and strain-gradient elasticity*. Physical Review B, 2016. **93**(24): p. 245107 <https://doi.org/10.1103/PhysRevB.93.245107>.
6. Mizzi, C.A. and L.D. Marks, *When Flexoelectricity Drives Triboelectricity*. Nano Lett, 2022 <https://doi.org/10.1021/acs.nanolett.2c00240>.
7. Olson, K.P., C.A. Mizzi, and L.D. Marks, *Band Bending and Ratcheting Explain Triboelectricity in a Flexoelectric Contact Diode*. Nano Lett, 2022 <https://doi.org/10.1021/acs.nanolett.2c00107>.

Enhancing liquid/solid interfacial energy to highlight the elasticity of mesoscopic liquids: long-range correlations and new thermodynamic effects

Laurence Noirez¹

¹*Laboratoire Léon Brillouin (CEA-CNRS), Université Paris-Saclay
CEA-Saclay, 91191 Gif-sur-Yvette Cedex, France*

On the basis of a Maxwell gas model, it has long been assumed that liquids are viscous in the hydrodynamic regime and exhibit (shear) elasticity at high sollicitation frequencies (MHz or GHz) only. By reinforcing the liquid/substrate interface interactions, recent experimental developments have proven that liquid exhibit also elasticity at very low frequency (\sim Hz); i.e. a “static” shear elasticity [1]. The shear elasticity is identified at mesoscopic scale, in both liquids and complex fluids (polymer melts, Van der Waals liquids, liquid water, H-bond liquids or physiological fluids) pointing out a generic character. As a result, liquids support the propagation of shear waves providing the liquid/surface interfacial conditions transmit the stress. New theoretical frameworks confirmed now the existence of a finite liquid shear elasticity [2,3]. It will be shown on some examples how the liquid elasticity has profound implications on flow, surface instabilities, thermodynamics, fluidic transport mechanisms and make possible the identification of new liquid properties like thermo-elasticity (Figure below)[4,5].

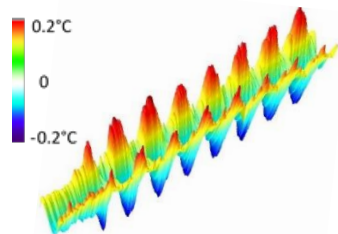


Figure 1: By applying a low frequency mechanical stimulus (\sim Hz), the liquid emits a modulated thermal signal synchronous with the stimulus (real-time mapping of the temperature of the PPG-4000 confined in a 240 μ m gap) [4,5].

- [1] L. Noirez, Importance of Interfacial Interactions to Access Shear Elasticity of Liquids and Understand Flow Induced Birefringence from Liquid Crystals to Worm-Like Micellar Solutions, *Oil & Gas Science and Technology – Rev. IFP Energies Nouvelles* 72, 10 (2017).
- [2] Zaccone, A.; Trachenko, K. Explaining the low-frequency shear elasticity of confined liquids. *PNAS*, 117, 19653–19655 (2020).
- [3] Alessio Zaccone and Laurence Noirez, Universal $G' \sim L^{-3}$ Law for the Low-Frequency Shear Modulus of Confined Liquids, *J. Phys. Chem. Lett.* 12, 1, 650–657 (2021).
- [4] E. Kume, P. Baroni & L. Noirez, Strain-induced violation of temperature uniformity in mesoscale liquids. *Scientific Reports* (2020) 10, 13340 doi: 10.1038/s41598-020-69404-1.
- [5] E. Kume, L. Noirez, Identification of Thermal Response of Mesoscopic Liquids under Mechanical Excitation: From Harmonic to Nonharmonic Thermal Wave, *J. Phys. Chem. B*, 125, 8652–8658 (2021).

Mesoscale organization in models of biological tissue

Austin Hopkins¹, Michael Chiang², Benjamin Loewe², Davide Marenduzzo², M. Cristina Marchetti¹

¹Department of Physics, University of California Santa Barbara, Santa Barbara, CA 93108, USA

²School of Physics and Astronomy, University of Edinburgh, Edinburgh, EH9 3FD, UK

In this talk I will describe recent work by my group and collaborators that employs multi-phase field models of motile cells on a frictional substrate to investigate the emergent mechanics of biological tissue. Using this model, we have examined the interplay between cell-cell and cell-environment interaction and dissipation in controlling the structure and rheology of tissue monolayers. The unperturbed tissue exhibits a transition between a solid-like state and a fluid-like state tuned by cell motility and cell deformability. When perturbed by a microrheological probe, solid tissues exhibit complex yield-stress behavior. Cell-cell dissipation can further drive mesoscale nematic order in the solid-liquid transition region. Our results point to new mechanisms for tuning collective cell dynamics in living tissue.

Energy dissipation in soft adhesion from a depinning perspective

Antoine Sanner and [Lars Pastewka](#)

lars.pastewka@imtek.uni-freiburg.de

Cluster of Excellence livMatS, University of Freiburg, Germany

Department of Microsystems Engineering, University of Freiburg, Germany

Understanding how roughness affects adhesion of soft solids is important for seals, skin adhesives and pick and place systems. In soft elastic contacts, surface roughness can trigger elastic instabilities which dissipate energy, leading to adhesion hysteresis without material-specific irreversibility. However, the role of these instabilities in adhesion hysteresis remains poorly understood because we lack theoretical and numerical models accounting for realistic roughness. Our work aims to build such a model focusing on the adhesion of soft elastic spheres with low roughness (Fig.1a), where the indentation process can be described as a Griffith-like propagation of a nearly circular external crack. The equilibrium position of the contact perimeter results from the competition between elastic deformation energy and local adhesion. Local fluctuations of the elastic deformation energy (resulting from roughness) create energy barriers leading to local instabilities. Local fluctuations of the work of adhesion (or fracture toughness) have a similar effect and we map the surface topography into an equivalent fracture toughness heterogeneity using weight-function theory [1]. This mapping allows us to describe the contact of rough spheres using efficient crack-perturbation simulations [2]. The crack-front model describes the adhesion of rough spheres as the pinning of an elastic line by a random potential, a generic problem that has already been studied in other contexts such as contact angle hysteresis and fracture of heterogeneous materials [3]. These previous theoretical results supplemented by our simulations show that the adhesion hysteresis is proportional to the elastic energy needed to flatten the self-affine random roughness, as long as this elastic energy is small enough for the contact area to remain nearly circular. We verify using the boundary-element method [4] that our crack-front model is accurate in this low roughness limit (Fig.1b).

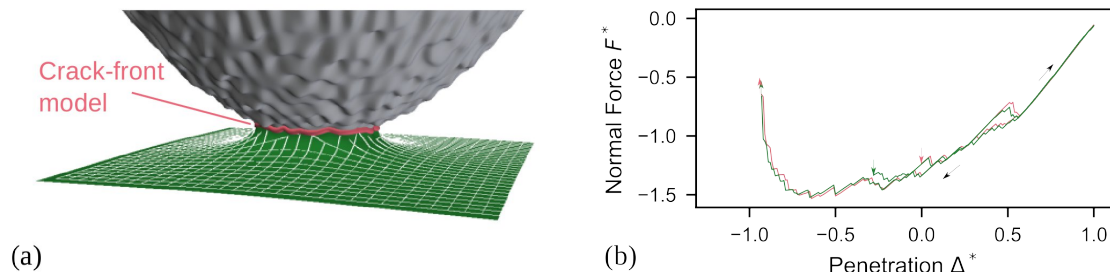


Figure 1: Adhesion of a rough sphere on an elastic halfspace. (b) The force penetration curve computed with the new crack-front model agrees with the boundary-element method (BEM).

References

- [1] J. R. Rice, Weight function theory for three-dimensional elastic crack analysis, in *Fracture mechanics: Perspectives and directions (Twentieth symposium)*, R. Wei, R. Ganglof., Eds., 29-57, 1989.
- [2] A. Sanner and L. Pastewka, Crack-front model for adhesion of soft elastic spheres with chemical heterogeneity, *J. Mech. Phys. Solids*, in press.
- [3] V. Démery, A. Rosso and L. Ponsón, From microstructural features to effective toughness in disordered brittle solids., *Europhys. Lett.* 105:34003, 2014.
- [4] L. Pastewka and M.O. Robbins, Contact area of rough spheres: Large scale simulations and simple scaling laws, *Appl. Phys. Lett.*, 108:221601, 2016.

Speaker: Seyedmehdi VAEZALLAEI (University of Tehran, Iran)

Friction of a self assembled structure at interface

Here, we study, the diffusivity of a self assembled structure on different interfaces, such as graphene and other 2D materials. We show how the immovability depends on the nano structure or potential pattern of interface.

Grain Boundary Sliding and Low Friction in Metals

Michael Chandross

Material, Physical and Chemical Sciences Center
Sandia National Laboratories, Albuquerque NM USA

The observed friction in metallic contacts is a direct result of the nanoscale mechanisms that accommodate plastic deformation. Previous work has demonstrated that for metals, low friction acts is associated with the formation and persistence of a thin layer of ultra-nanocrystalline material (i.e., with grain sizes less than about 10 nm) at the sliding interface. At these grain sizes, shear is no longer accommodated by the creation and motion of dislocations, but rather through grain boundary sliding, in a manner similar to the softening observed in the inverse Hall-Petch regime. We present a theoretical treatment of grain boundary sliding that provides both a qualitative and quantitative description of low friction in metallic contacts. This framework -- based purely on materials properties with no adjustable parameters -- accurately predicts the strength of a variety of metals, including pure FCC, BCC, and HCP systems, as well as dilute alloys and metallic glasses. These calculations also imply fundamental limits on the lowest achievable friction coefficients in metals. By directly connecting interatomic bond strengths and nanoscale deformation mechanisms with the macroscale properties of metals, this work implies opportunities for the optimization of metal alloys for both low friction and high strength applications.

This work was funded by the Laboratory Directed Research and Development program at Sandia National Laboratories, a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Speaker: AIAlejandro JENKINS VILLALOBOS (International Centre for Theory of Quantum Technologies (ICTQT), Poland)

Quantum theory of triboelectricity

We propose a microphysical theory of the triboelectric effect by which mechanical rubbing separates charges across the interface between two materials. Surface electrons are treated as an open system coupled to two baths, corresponding to the bulks. Extending Zeldovich's theory of bosonic superradiance, we show that motion-induced population inversion can generate an electromotive force. We argue that this is consistent with the basic phenomenology of triboelectrification and triboluminescence as irreversible processes, and we suggest how to carry out more precise experimental tests. This work has been published as: R. Alicki and A. Jenkins, *Phys. Rev. Lett.* 125, 186101 (2020).

Trajectory Anisotropy of a Sliding Tip Induced by Apex Asymmetry

Ai Sadeghi¹

¹*Department of Physics, Shahid Beheshti University, Tehran, Iran*

When the sharp tip of a scanning probe microscope is dragged on a perfect crystalline surface, crystallographic equivalent directions might seem to show the same friction patterns and dissipation behaviour. However, this is not the case if the tip apex is not structureless. We quantify the difference between the energy dissipation when the tip is dragged in opposite directions along a given scan line by simulation. The same is shown for other equivalent directions on the surface. When the tip apex is modelled with a small silicon cluster, the simulation results fit the experimentally observed asymmetry for forward and backward scans along a given scan orientation on NaCl(001) surface at room temperature [1]. The traditional Prandtl-Tomlinson model fails to explain the difference of the energy dissipation in opposite directions. We adapt the model by replacing the sinusoidal corrugation potential with our own *ab initio* based interaction potential which takes into account the apex atomic structure while both atomic and electronic relaxations of the tip apex in response to the interaction with the sample surface are considered. Then the dissipation difference is attributed to the direction dependent tip-apex trajectory. This is in perfect agreement with the experimentally captured trajectory of the tip. The effect of the tip-apex sharpness, the stiffness of the tip body-cantilever complex, temperature and the normal load on the trajectory anisotropy and energy dissipation are investigated in detail. Interestingly, the dominant factor is shown to be the apex atomic structure.

[1] G. Fessler, A. Sadeghi, T. Glatzel, S. Goedecker, E. Meyer, Tribol. Lett. **67**, 59 (2019)

Interlayer electronic transport in sheared bilayer graphene systems

Elad Koren

Faculty of Materials science & engineering, Technion – Israel Institute of Technology, Haifa, Israel.

eladk@technion.ac.il

Weak interlayer coupling in 2-dimensional layered materials such as graphene gives rise to rich mechanical and electronic properties, in particular in the case where the two atomic lattices at the interface are rotated with respect to one another. The reduced crystal symmetry leads to anti-correlations and cancellations of the atomic interactions across the interface, leading to low friction¹ and low interlayer electrical transport². Using our recent nanomanipulation technique, based on atomic force microscopy, we show that combined electro-mechanical characterization can uniquely address open fundamental questions related to electronic charge transport²⁻³ through stacking faulted structures. To this end, we studied experimentally and theoretically the interlayer charge transport in twisted bilayer graphene systems separately for edges and bulk parts. We find that interlayer edge currents are several orders of magnitude larger than in the bulk and therefore govern the transport up until very large critical diameters depending on the potential across the adjacent layers and the angular mismatch angle³. In addition, we show that the strong edge transport across the interface is governed by strong quantum mechanical interference effects as opposed to simple interlayer atomic interactions⁴.

[1] E. Koren *et al.*, *Science*, 6235 (2015) 679.

[2] E. Koren *et al.*, *Nature Nanotech.*, 9 (2016) 752.

[3] D. Dutta *et al.*, *Nature Comm*, 11 (2020) 4746.

[4] A. Oz *et al.*, *Advanced Science*, (2022), in press.

Friction, wear, lubrication and tribochemical reactions using in situ atomic force microscopy in liquids

Nitya Nand Gosvami

Department of Materials Science and engineering, Indian Institute of Technology, Hauz Khas, New Delhi-110016, India

Abstract

Controlling friction and wear is crucial for reducing energy and material losses, harmful emissions, and improving the reliability of various engineering components. However, the complexities at the buried sliding interfaces under dry as well as lubricated conditions require deep scientific understanding to unravel the physical mechanisms controlling friction and wear. Atomic force microscopy (AFM) is a powerful tool to address a few of these challenges as it greatly simplifies the geometry of the sliding interfaces and allows nanoscale single-asperity level investigation of friction and wear. Based on an in situ AFM based approach, I'll discuss monitoring of tribochemical reaction under lubricated sliding contacts, resulting in robust tribofilm formation from commercial antiwear additive zinc dialkyldithiophosphate (ZDDP), mixed with the base oil. Experiments performed on various material combinations show that the reaction is driven by stress and temperature and provide valuable information on multiphase alloys of Al and Mg where the contribution of individual chemically and mechanically distinct regions on tribofilm growth can be investigated with unprecedented resolution. It is observed that the tribofilms preferentially form on hard precipitate regions whereas significant wear of soft Al and Mg matrix regions occur. Amide based additives reveal significantly better tribofilm growth characteristics as well as substantially lower friction than ZDDP for Mg-based alloys. For Al-based alloys (e.g., ADC12), combination of ZDDP with oil dispersed hexagonal boron nitride (hBN) promotes growth of antiwear tribofilm on Al matrix regions as well as reduced friction.

Structural Superlubricity: From Dissipation to Functioning

Quanshui Zheng^{1,2}, Ming Ma^{1,2}, Zhiping Xu^{1,2}

¹Center for Nano and Micro Mechanics, Tsinghua University, Beijing 100084, China

²Institute of Superlubricity Technology, Research Institute of Tsinghua University in Shenzhen, Shenzhen 518057, China

Structural superlubricity (SSL) is a state of ultralow friction and zero wear between two solid surfaces in direct contact sliding with respect to each other. In this talk, we will first discuss the mechanisms of SSL based on our recent experimental and theoretical works, with focusing on the origin of energy dissipation or friction as well as the robustness of SSL. The broader aspect of SSL-derived science and technology will then be outlined and exemplified by prototypical electromechanical devices. Last but not least, we will show our latest progresses in pushing SSL towards practical applications, including various functioning devices such as nanogenerators, RF MEMS and slip rings.



Dissipation Mechanisms in Nano/Mesoscale Tribological Systems | (SMR 3713)

POSTER SESSION 'IN PERSON' on 30 MAY 2022 at 18:00 CEST

| | |
|---------------------------------------|--|
| P01 - ALIASGARI Mojgan | Sliding Friction of Wet Granular Media |
| P02 - CHEN Yun | Spatial Separation of Enantiomers by Field-Modulated Surface Scattering |
| P03 - CIHAN Ebru | Multi Contact Friction of Laser Induced Periodic Surface Structures (LIPSS) on Stainless Steel |
| P04 - CREMASCHINI Sebastian | Optofluidic Platform for the Manipulation of Water Droplets on Engineered LiNbO ₃ Surfaces |
| P05 - GIANETTI Melisa Mariel | Thermal Friction Enhancement and Electric-Field Effects in Zwitterionic Monolayers |
| P06 - HAREA Evghenii | Mullins effect in rubber friction |
| T07 - SILVA Andrea | Design principles for crystalline interfaces: directional locking, directional superlubricity and structural lubricity |
| P08 - SONG Yiming | Nanotribological properties of MoS ₂ on Au(111) in ultrahigh vacuum |
| P09 - SPASOV Hristov Georgi | Simulation of pharmaceutical aerosols deposition in human lungs |
| P10 - STANKOVIC Igor | Nature of dynamic friction in a humid hydrophobic nanocontact |
| P11 - ZAMBUDIO SEPÚLVEDA Aitor | Fine Defect Engineering of Graphene Friction |

POSTER SESSION VIRTUAL (ZOOM) on 1 JUNE 2022 at 18:00 CEST

| | |
|--|---|
| P01 (Zoom) - CAO Wei | Energy dissipation in a finite two-dimensional monolayer |
| P02 (Zoom) - DJOUMKAM MOUAFO Maelle Laure | Anisotropie de friction des structures de bisulfure de molybdène et du graphite à l'échelle nanométrique |
| P03 (Zoom) - JIMIDAR Ignaas | Self-organization of horizontally agitated microspheres |
| P04 (Zoom) - MAZO TORRES José Juan | Ripple formation and evolution in compliant materials |
| P05 (Zoom) - MOVAHEDI Behrooz | Tribological study of Fe-Based Amorphous Nanocomposite Coatings Reinforced by B ₄ C Nanoparticles |
| P06 (Zoom) - MUGWANEZA Denyse | DEVELOPMENT OF ACTIVATED CARBON FROM WASTE |
| P07 (Zoom) - RYAZANOV Vasyi Vasyi | Effect of entropy changes on time to failure caused by tribological causes |
| P08 (Zoom) - SHAH Hussain Wiqar | Magnetic spin losses, Competing Interactions, and magnetization dynamics in Doped Rare-earth Manganites nanostructural system |
| P09 (Zoom) - VERNES Andrés | Frictional dissipation in the 2D Prandtl-Tomlinson model |

Sliding Friction of wet granular media

Moigan Aliasgari¹, Nahid Maleki-Jirsaraei¹, and Shahin Rouhani²

¹ *Complex Systems Laboratory, Physics Department, Alzahra University, P.O. Box 1993891176, Tehran, Iran*

² *Physics Department, Sharif University of Technology, P.O. Box 11155-9161, Tehran, Iran*

Energy loss due to friction is a well-known characteristic of granular materials. The mechanical response of sand is largely dominated by the amount of water added to it [1]. Adding a small amount of water to sand increases the hardness which results in a decrease of the sliding friction [2]. Pouring even more water to sand results in a decrease of the hardness and a subsequent increase of the friction. This inverse correlation between hardness of a wetted granular material and its frictional response to sliding is found to be due to ploughing of the sledge.

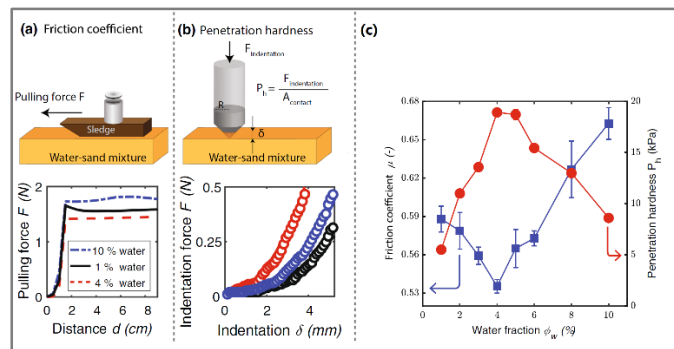


Fig. 1 Schematic representation and corresponding curves of the sliding experiment (a) and hardness test (b). (c) Evolution of the friction coefficient μ (blue squares) and the penetration hardness P_h (red circles) for the water volume fraction Φ_w .

Our results show the influence of grains characteristics (size and shape) and properties of interstitial liquid (surface tension and viscosity).

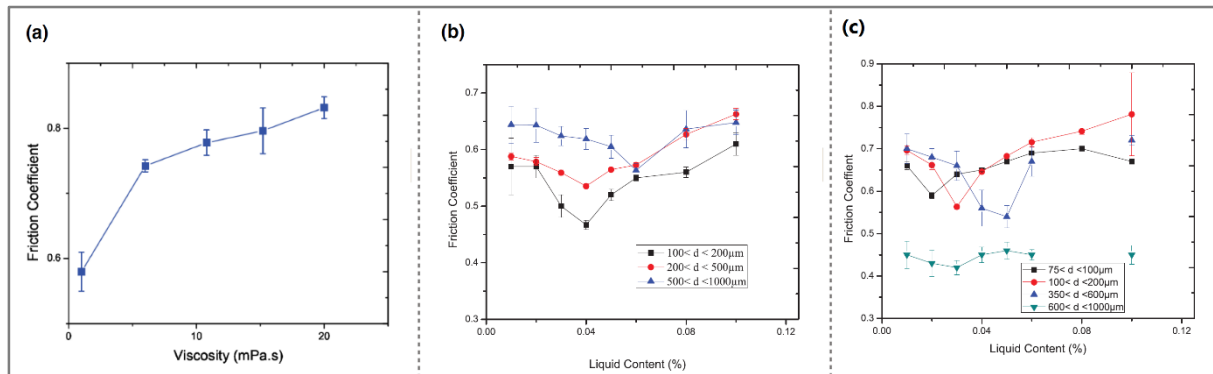


Fig. 2 (a) Dynamic friction coefficient vs viscosity for water and glycerol mixture as the interstitial liquid in the sand. The volume fraction of the interstitial liquid (mixtures of pure water and glycerol) is fixed at 3% for all experiments. Dynamic friction coefficient vs. volume fraction of interstitial liquid for (b) sand and water and (c) glass beads and silicone oil [3]

Earlier experiments were limited to low-viscosity liquids such as water and low-viscosity silicone oil. It was shown that viscosity also plays a role in the dynamic mechanical properties of wet granular matter.

[1] P. C. F. Moller, D. Bonn, *Europhys. Lett.* **80**, 38002 (2007).

[2] R.W. Liefferink, M. Aliasgari, N. Maleki-Jirsaraei, S. Rouhani, D. Bonn, *Granul. Matter* **22**, (2020).

[3] M. Aliasgari, N. Maleki-Jirsaraei, S. Rouhani, *Z Phys Chem*, (2019).

Spatial Separation of Enantiomers by Field-Modulated Surface Scattering

Yun Chen, Oded Hod, and Michael Urbakh

*Department of Physical Chemistry, School of Chemistry, The Raymond and Beverly Sackler Faculty of Exact Sciences, Tel Aviv University,
Tel Aviv 6997801, Israel*

Molecular chirality is of fundamental importance in chemistry and biology and may hold the key to deciphering the enigmatic puzzle of the origin of life [1]. Despite its great significance, challenges remain in enantioseparation [2-4]. Herein, a novel strategy for spatial separation of different enantiomers with nonzero permanent dipole moment is proposed based on mechanical chiral resolution. We theoretically demonstrate that by partially pre-orienting chiral molecules with the help of a linearly polarized laser pulse in conjunction with a strong time-delayed homogeneous static electric field, a chiral field can be introduced to make the frictional surface scattering of different enantiomers in the opposite direction. Relying on classical molecular dynamics simulations, we find that friction determines the enantioseparation, where the electrostatic field-induced dipole orientation plays a central role in achieving a chiral field while the pulse-triggered molecular alignment contributes to the higher quality of the chiral field. Remarkably, the excellent agreement with quantum mechanical results confirms the classical nature of excitation methods, suggesting the operational robustness of this enantioseparation approach. Furthermore, because of the uncovered minor side effect of molecular deformation on enantioseparation, thoroughly numerical simulations promise this approach the feasibility and high efficiency in practical applications. It is noteworthy that terahertz (THz) pulses have recently been proven to facilitate the classical dipole orientation [5]. Thus, the use of THz pulses instead of the electrostatic fields allows for all-optical field-free modulation of this enantioseparation approach.

- [1] W. A. Bonner, *Chirality and Life*, Orig. Life Evol. Biosph. **25**, 175 (1995).
- [2] I. Agranat, H. Caner, and J. Caldwell, *Putting Chirality to Work: The Strategy of Chiral Switches*, Nat. Rev. Drug Discov. **1**, 753 (2002).
- [3] T. J. Ward and K. D. Ward, *Chiral Separations: A Review of Current Topics and Trends*, Anal. Chem. **84**, 626 (2012).
- [4] V. Marichez, A. Tassoni, R. P. Cameron, S. M. Barnett, R. Eichhorn, C. Genet, and T. M. Hermans, *Mechanical Chiral Resolution*, Soft Matter **15**, 4593 (2019).
- [5] L. Xu, I. Tutunnikov, E. Gershnel, Y. Prior, and I. S. Averbukh, *Long-Lasting Molecular Orientation Induced by a Single Terahertz Pulse*, Phys. Rev. Lett. **125**, 13201 (2020).

Multi-Contact Friction of Laser-Induced Periodic Surface Structures (LIPSS) on Stainless Steel

Ebru Cihan¹, John Heier², Stephan Gräf², Frank A. Müller², Enrico Gnecco^{1,3}

¹*Chair of Materials Science and Nanotechnology, Technical University Dresden, 01069 Dresden, Germany*

²*Otto Schott Institute of Materials Research (OSIM), Friedrich Schiller University Jena, 07743 Jena, Germany*

³*Marian Smoluchowski Institute of Physics, Jagiellonian University, 30-348 Krakow, Poland*

Despite many advances in the fundamentals of nanotribology, friction processes at larger scales are poorly understood, since the material and geometrical features of multi-asperity contact surfaces change as they slide over each other. In this contribution, we present the results of AFM measurements on the friction dynamics of sliding contacts formed by colloidal AFM probes and (rough) laser-induced periodic surface structures (LIPSS). Polymethyl methacrylate (PMMA) microspheres have been scanned parallel and perpendicular to LIPSS on stainless steel. Depending on the ratio between the sphere diameters and the LIPSS periods, the friction response is governed either by the topographic convolution of the two surfaces in contact or by the stick-slip motion on the background of the LIPSS roughness (independently of the scan direction). We have also investigated the influence of the AFM feedback gain by progressively changing the scan conditions from constant load to constant height while sliding. Our results extend preliminary investigations on periodic wedge-shaped microgratings [1]. The ultimate goal is to shed light on the mechanisms of tactile perception in both living organisms and artificial sensors.

[1] A. Özogul, S. Gräf, F. A. Müller, E. Gnecco, Trib. Lett. **67** 29 (2019).

Abstract template for poster

Optofluidic Platform for the Manipulation of Water Droplets on Engineered LiNbO₃ Surfaces

Sebastian Cremaschini¹, Annamaria Zaltron¹, Davide Ferraro¹, Alessio Meggiolaro¹, Mattia Carneri¹, Enrico Chiarello¹, Paolo Sartori¹, Matteo Pierno¹, Cinzia Sada¹ and Giampaolo Mistura¹

¹*Dipartimento di Fisica ed Astronomia "Galileo Galilei", Università di Padova, Via Marzolo 8, 35131 Padova (Italy)*

The actuation and control of liquid droplets on a surface have important implications in many industrial applications and microfluidics. Reproducible motion of water droplets on a solid surface is very difficult to achieve because of the presence of surface defects. Bioinspired liquid-infused surfaces (LISs), made of textured materials imbibed with a low surface tension oil [1], exhibit various unique properties attributed to their liquid-like and molecularly smooth nature. In particular, they enable low friction droplet motion [2].

We have realized LISs by impregnating a porous Teflon filter with a fluorinated oil using a dip-coater to ensure high reproducibility. This process allows one to obtain very slippery hydrophobic surfaces for prolonged use [3]. Their performances are tested by analyzing the motion and speed of repeated sequences of water droplets with different volumes and deposited on a sample tilted at different angles; it is found that the LIS can be used safely for the motion of thousands of droplets (about a week of laboratory use).

In this work, droplet actuation is achieved by exploiting the photovoltaic effect of iron-doped lithium niobate (LiNbO₃): when the crystal is illuminated, surface charges of opposite sign are generated on the two faces of the crystal [4]. The face of LiNbO₃ in contact with the droplets is coated with the LIS to create a low friction surface: in this way sessile water droplets having volumes of microliters, corresponding to millimeters in size, can be easily actuated, guided, merged and split by projection on the crystal of suitable static or dynamic light patterns (see **Figure 1**) The actuated droplets can cover distances of centimeters on a timescale of a few seconds [5].

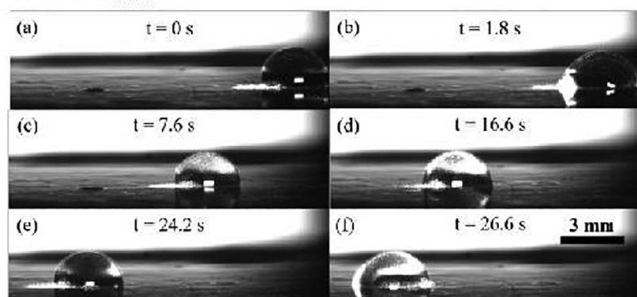


Figure 1: Sequential video frames showing the motion of a water droplet along a pattern constituted by circular spots, illuminating different regions of the sample.

- [1] T.-S. Wong et al., *Nature* **477**, 443-447 (2011).
- [2] J.D. Smith et al., *Soft Matter* **9**, 1772-1780 (2013).
- [3] P. Sartori et al., *Commun. Phys.* **5**, 10.1038/s4 (2022).
- [4] A. Puerto et al., *Phys. Rev. Appl.* **13**, 24046 (2020).
- [5] A. Zaltron et al., submitted to *Adv. Mater. and Interf.*

Thermal Friction Enhancement in Zwitterionic Monolayers

Melisa M. Gianetti¹, Roberto Guerra², Andrea Vanossi^{3,4}, Michael Urbakh⁵ and Nicola Manini¹

¹*Dipartimento di Fisica, Università degli Studi di Milano, Via Celoria 16, Milano, 20133 Italy*

²*Center for Complexity and Biosystems, Department of Physics, University of Milan, via Celoria 16, Milano, 20133, Italy*

³*CNR-IOM, Consiglio Nazionale delle Ricerche - Istituto Officina dei Materiali, c/o SISSA, Via Bonomea 265, 34136 Trieste, Italy*

⁴*International School for Advanced Studies (SISSA), Via Bonomea 265, 34136 Trieste, Italy*

⁵*Department of Physical Chemistry, School of Chemistry, The Raymond and Beverly Sackler Faculty of Exact Sciences and The Sackler Center for Computational Molecular and Materials Science, Tel Aviv University, Tel Aviv 6997801, Israel*

We introduce a model for zwitterionic monolayers and investigate its tribological response to changes in applied load, sliding velocity, and temperature by means of molecular-dynamics simulations. The proposed model exhibits different regimes of motion depending on temperature and sliding velocity. In particular, in confined geometries, friction is affected by temperature, usually exhibiting a regular “thermolubric” behavior, with friction decreasing as temperature increases at microscopic scales [1-3]. The rationale for this standard behavior is random thermal fluctuations assisting the sliding interface in the negotiation of interlocking barriers, thus promoting advancement. The reverse, namely, friction increasing with temperature, is far less common, although it has been observed in specific situations [4-6].

In our simulations, we find a remarkable increase of friction with temperature, which we attribute to the formation and rupture of transient bonds between individual molecules of opposite sliding layers, triggered by the out-of-plane thermal fluctuations of the molecules’ orientations. To highlight the effect of the molecular charges, we compare these results with analogous simulations for the charge-free system.

Our findings are expected to be relevant to nanoscale rheology and tribology experiments of locally-charged lubricated systems such as, e.g., experiments performed on zwitterionic monolayers, phospholipid micelles, or confined polymeric brushes in a surface force apparatus.

We will also show the effect on friction when these zwitterionic monolayers are exposed to an external electric field.

[1] Y. Sang, M. Dubé, M. Grant, *Phys. Rev. Lett.* **87**, 174301 (2001).

[2] O. M. Dudko, A. Filippov, J. Klafter, M. Urbakh, *Chem. Phys. Lett.* **352**, 499 (2002).

[3] P. Steiner, R. Roth, E. Gnecco, A. Baratoff, S. Maier, T. Glatzel, E. Meyer, *Phys. Rev. B* **79**, 045414 (2009).

[4] A. Vanossi, D. Dietzel, A. Schirmeisen, E. Meyer, R. Pawlak, T. Glatzel, M. Kisiel, S. Kawai, N. Manini, *Beilstein J. Nanotechnol.* **9**, 1995 (2018).

[5] I. Barel, M. Urbakh, L. Jansen, A. Schirmeisen, *Phys. Rev. Lett.* **104**, 066104 (2010).

[6] J. Zhu, Q. Zeng, Y. Wang, C. Yan, W. He, *Tribol. Lett.* **68**, 50 (2020).

Mullins effect in rubber friction

E. Harea¹

¹ *Institute of Applied Physics, Academy of Sciences of Moldova*

The present study focuses on newly observed rubber swelling detected in contact region of reciprocated ball-on-flat friction test. Flat Natural Rubber (NR) samples unfilled and filled with Carbon Black (CB) were subjected to 50 cycles of sliding friction, repeated for different normal forces. For all testing conditions swelling gradually increased in first 5-6 cycles, followed by a steady state stage, affected later by wear development. Bigger normal force led to bigger swelling. Such a rubber comportment during reciprocating friction test was considered by us as a consequence of Mullin's effect [1]. It was noticed the direct relation between swelling growth and friction coefficient decrease. Finally, was briefly discussed the influence of initial rubber deformation during static loading on later sliding trajectory.

[1] L. Mullins, Effect of stretching on the properties of rubber, J. Rubber Res. **16** (1947), pp. 275-289

Title: Design principles for crystalline interfaces: directional locking, directional superlubricity and structural lubricity

Abstract: Friction at nanoscale shows a wide range of phenomena from high-friction stick-slip motion to superlubricity and directional locking. At this length scales, the friction is largely dependent on the atomic arrangement of crystalline structures at the two contacting surfaces. Given an arbitrary interface, i.e. two mutually rotated 2D lattices, what is the qualitative friction behaviour to expect?

We qualify the friction regimes solely on geometrical consideration, both in the infinite-size limit and for finite-size adsorbate. We calculate the interlocking potential energy of a rigid monolayer crystal in contact with a rigid periodic surface. Analytical theory is consistent with numerical simulation and colloidal experiments. The novel regime of directional superlubricity provides the potential to design nanoscopic high-speed rails with frictionlessly sliding along engineered directions.

Nanotribological properties of MoS₂ on Au(111) in ultrahigh vacuum

Yiming Song, Antoine Hinaut, Sebastian Scherb, Yves Pellmont, Rémy Pawlak, Zhao Liu, Thilo Glatzel, and Ernst Meyer

Department of Physics, University of Basel, 4056 Basel, Switzerland

Molybdenum disulfide (MoS₂), a single layer of Mo atoms sandwiched in between two layers of S atoms, shows a wide range of potential applications in the fields of electronics, optoelectronics and micro and nanomechanical systems requiring ultralow friction[1,2]. Due to its superior structural and mechanical characteristics, strong in-plane covalent bonding combined with weak interlayer van der Waals interaction, MoS₂ has been used as solid lubricant especially in aerospace applications[3].

The structural and superlubric properties of single layer MoS₂ on Au(111) forming moiré structures have been investigated by means of ultrahigh vacuum atomic force microscopy with bimodal and contact modes. We grow monolayer MoS₂ flakes on an Au(111) surface having a hexagonal superstructure of patches with ~45 pm corrugation and about ~3.3 nm periodicity. Friction force microscopy measurements at the atomic scale indicate a superlubric regime between the tip apex and the MoS₂ surface in which the friction force remains at an ultralow value and is independent from normal load. Superlubricity conditions are observed for different loads and velocities which indicates the absence of out-of-plane deformations. We do find that the MoS₂ layer including the moiré superlattice modulation originating from the natural misfit between MoS₂ and the Au(111) substrate is relatively rigid. We also demonstrate a nonmonotonic frictional speed dependence of the MoS₂ surface induced by multi-slip effect. Our results open up a new avenue for minimizing friction in nanoscale electronic devices and other dry rigid contacts used in aerospace lubrication.

[1] Geim, A. K. et al., Nature 499, 419–425 (2013)

[2] Hod, O. et al., Nature 563, 485–492 (2018)

[3] Roberts, E. W., J. Phys. D-Appl. Phys. 45, 503001 (2012)

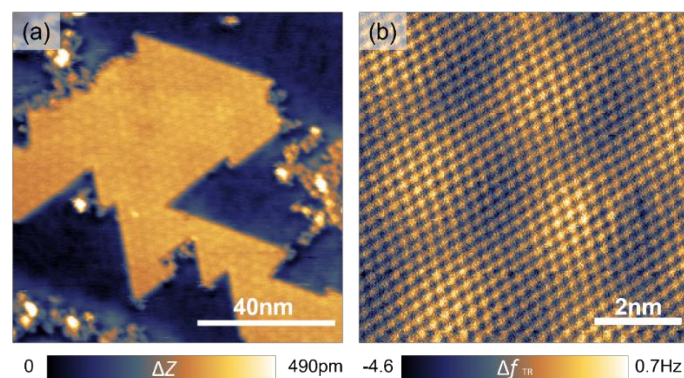


Fig 1. (a) 100 nm × 100 nm topographic nc-AFM image of a single layer MoS₂ flake. (b) High-resolution image showing the moiré and the atomic structure of the MoS₂ islands in the torsional frequency shift Δf_{TR} recorded in bimodal AFM. Parameters: (a) $\Delta f_{1st} = -10$ Hz, $A_{1st} = 2.5$ nm, (b) $\Delta f_{2nd} = -100$ Hz, $A_{2nd} = 800$ pm, $A_{TR} = 80$ pm.

Simulation of pharmaceutical aerosols deposition in human lungs

G.H. Spasov^{1,3}, R.Rossi⁴, A.Vanossi^{1,3}, C.Cottini², and A. Benassi^{1,2}

¹*International School for Advanced Studies (SISSA), Trieste (Italy) 1*

²*Chiesi Farmaceutici S.p.A, Parma(Italy)*

³*CNR-IOM, Consiglio Nazionale delle Ricerche - Istituto Officina dei Materiali, c/o SISSA, Via Bonomea 265, 34136, Trieste, Italy*

⁴*RED Fluid Dynamics, Via Pompeo Bevitori 4, 47876 Talamello (RN) ,Italy*

The possibility to use computational fluid dynamics (CFD) techniques to study the behaviour of air and airborne aerosol particles in realistic airways geometries has attracted a lot of attention in the last two decades. Improving our understanding of particles transport and deposition in such complex flows is of significant importance in the development/optimization of orally inhaled drug products. Despite the great variety and quantity of works and reviews on the subject [1]–[5], there are no common criteria for the reliability assessment of these simulations. With the present work, we aim at presenting a critical analysis of various technical aspects strongly influencing the simulation results and thus their overall reliability and exploitability for industrial applications. A critical overview of the numerical aspects, e.g. mesh sensitivity analysis, and of the main physical ingredients, e.g. time dependent fluctuations, turbulent dissipation, is presented along with their effects on particle dynamics and deposition.

- [1] J. Tu, K. Inthavong, and G. Ahmadi, *Computational Fluid and Particle Dynamics in the Human Respiratory System*. Dordrecht: Springer Netherlands, 2013. doi: 10.1007/978-94-007-4488-2.
- [2] H. Sierra, M. Cordova, C.-S. J. Chen, and M. Rajadhyaksha, “Confocal Imaging–Guided Laser Ablation of Basal Cell Carcinomas: An Ex Vivo Study,” *Journal of Investigative Dermatology*, vol. 135, no. 2, pp. 612–615, Feb. 2015, doi: 10.1038/jid.2014.371.
- [3] M. S. Islam, G. Paul, H. X. Ong, P. M. Young, Y. T. Gu, and S. C. Saha, “A Review of Respiratory Anatomical Development, Air Flow Characterization and Particle Deposition,” *International Journal of Environmental Research and Public Health*, vol. 17, no. 2, p. 380, Jan. 2020, doi: 10.3390/ijerph17020380.
- [4] P. W. Longest and L. T. Holbrook, “In silico models of aerosol delivery to the respiratory tract — Development and applications,” *Advanced Drug Delivery Reviews*, vol. 64, no. 4, pp. 296–311, Mar. 2012, doi: 10.1016/j.addr.2011.05.009.
- [5] Y. Feng, Z. Xu, and A. Haghnegahdar, “Computational Fluid-Particle Dynamics Modeling for Unconventional Inhaled Aerosols in Human Respiratory Systems,” in *Aerosols - Science and Case Studies*, InTech, 2016. doi: 10.5772/65361.

Nature of dynamic friction in a humid hydrophobic nanocontact

Olivier Noël^{1)*}, Pierre-Emmanuel Mazeran²⁾, and **Igor Stanković**^{3)†}

¹⁾ *IMMM, UMR CNRS 6283, Le Mans Université,*

Av. O. Messiaen, 72085 cedex 09, Le Mans, France

²⁾ *Sorbonne universités, Université de Technologie de Compiègne, UMR CNRS 7337, Roberval, Centre de recherche de Royallieu – CS 60319-60203 Compiègne cedex, France*

³⁾ *Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade, University of Belgrade, 11080 Belgrade, Serbia*

**Corresponding authors: * olivier.noel@univ-lemans.fr, † igor.stankovic@ipb.ac.rs*

The physics of dynamic friction on water molecule contaminated surfaces is still poorly understood. In line with the growing interest in hydrophobic contact for industrial applications, this paper focuses only on friction mechanisms in such interfaces. As a commonly used material, contact with graphite is considered in a twin-fold approach based on experimental investigations using an atomic force microscopy technique combined with molecular dynamic simulations.

AFM circular mode, used in this study, represents a novel experimental approach that provides a strictly controlled velocity and distance overextended sliding paths, see Fig. 1(a). This mode leads to a relative motion of the contact, without acceleration, deceleration, and any rest periods during sliding which necessarily occur with the conventional back and forth scanning mode. Our results demonstrate that a droplet may form by the accumulation of the adsorbed water (as a packman swallowing smaller water droplets) and stay within the sliding hydrophobic nanocontact, see Fig. 1(b). Then, the nature of the dynamic friction mechanism has been elucidated by considering the resistance of the water droplet driven by one side of the moving contact. We demonstrate that an intuitive paradigm must be refined, which asserts that water molecules are squeezed out of a hydrophobic contact. As a consequence, we introduce a new mechanism considering a droplet produced within the sliding nano-contact by the accumulation of water adsorbed on the substrate. Hence, our findings highlight new routes for controlling water-mediated friction in the air.

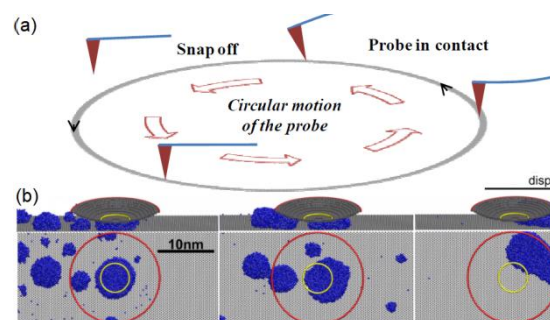


Fig 1. (a) Circular mode coupled with the adhesion force/coefficient of friction spectra. (b) Accumulation of adsorbed water on moving hydrophobic substrate. Distance between successive images is 10nm, $v=1\text{m/s}$.

[1] O. Noël, P.-E. Mazeran, I. Stanković, **Nature of dynamic friction in a humid nanocontact, submitted**

Fine Defect Engineering of Graphene Friction

A. Zambudio^{1,2}, **E. Gnecco**³, **J. Colchero**¹, **R. Pérez**^{4,5}, **J. Gómez-Herrero**^{2,5} and **C. Gómez-Navarro**^{2,5}

¹ *Optics and Nanophysics Research Center, Universidad de Murcia, Murcia, Spain*

² *Condensed Matter Physics Dept., Universidad Autónoma de Madrid, Madrid, Spain*

³ *Otto Schott Institute of Materials Research, Friedrich Schiller University of Jena, Germany*

⁴ *Theory Condensed Matter Physics Dept., Universidad Autónoma de Madrid, Madrid, Spain*

⁵ *Condensed Matter Physics Center, Universidad Autónoma de Madrid, Madrid, Spain*

Two-dimensional (2D) materials, in particular graphene, displays low friction coefficient and good wear properties. However, the very frequent presence of defects highly influences the friction and other mechanical properties of graphene. Tribological studies of defective graphene up to date combine coexistent substitution and vacancy-like defects with different sizes[1], hindering a fundamental understanding of the role of defects on graphene friction. In this work, we quantify the influence of controlled-induced monoatomic vacancies in graphene tribology using Atomic Force Microscopy (AFM). This simplest and very common defect demonstrated to very efficiently enhance the friction coefficient of graphene, yielding a 5-fold increase with a very low defect density, below 0.1% [2]. At the atomic-scale, we resolve monoatomic vacancies in friction force images showing a great correlation with Prandtl-Tomlinson model atomistic simulations.

Thorough analysis of real-space distribution of friction data at the nanoscale reveals two main contributions to friction enhancement. One is related to reactivity of dangling bonds localized at monovacancy site ($\sim 1\text{nm}^2$) and is responsible of $\sim 20\%$ of the increase. The other extends up to $\sim 25\text{nm}^2$ and arises from the long-range strain distribution around vacancies[3], being the main contribution to friction enhancement on defective graphene. These results elucidate the subtle connection between friction, reactivity, and mechanical properties in 2D materials.

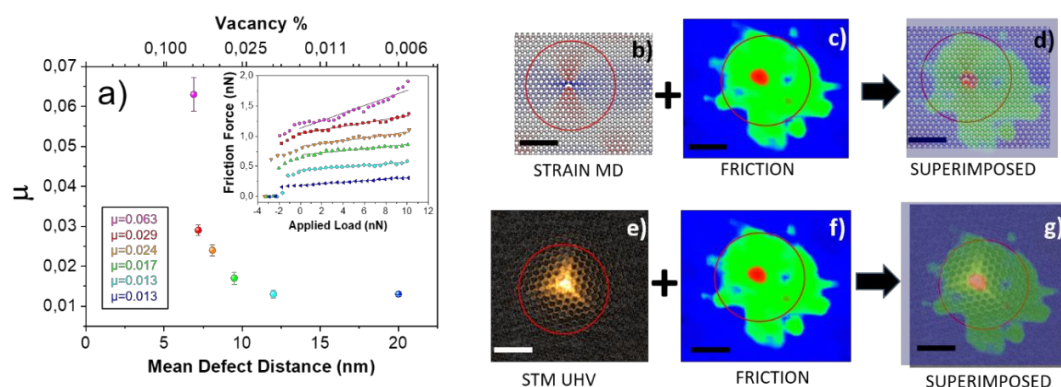


Fig.1: a) Friction coefficient vs mean defect distance. Inset: Friction force vs applied load curves from where friction coefficients are extracted. b)-g) Comparison of spatial distribution of monovacancy friction (c) and (f) with molecular dynamics strain simulations (b) and UHV STM image (e)

[1] S. Kwon, J-H. Ko, K-J. Jeon, Y-H. Kim, J. Y. Park, *Nano Lett.* **12** 6043-6048 (2012).

[2] A. Zambudio, E. Gnecco, J. Colchero, R. Pérez, J. Gómez-Herrero, C. Gómez-Navarro, *Carbon* **182** (2021).

[3] G. López-Polín, M. Ortega, G. Vilhena, I. Alda, J. Gómez-Herrero, P. A. Serena, C. Gómez-Navarro, R. Pérez, *Carbon* **116**, 670-677 (2017).

Dissipation Mechanisms in Nano/Mesoscale Tribological Systems | 30 May - 2 June,
Italy

Energy dissipation in a finite two-dimensional monolayer

Wei Cao, Oded Hod, and Michael Urbakh

School of Chemistry, The Raymond and Beverly Sackler Faculty of Exact Sciences and The Sackler Center for Computational Molecular and Materials Science, Tel Aviv University, Tel Aviv 6997801, Israel

The emerging of structural superlubricity in contacts of two dimensional (2D) materials attracts widely attention in recent decades. However, the mechanisms of frictional energy dissipation in finite incommensurate contacts still remain unclear. The previous model results obtained using e.g. the Frenkel-Kontorova-Tomlinson (FKT) model often depend on a value of damping coefficient, which is introduced to describe a dissipation of kinetic energy to internal degrees of freedom. The understanding of basic questions, such as the effect of contact size and sliding velocity on friction forces is still lacking.

A simple and tractable approach proposed in previous publications¹ provides a good starting point for understanding routes of energy transfer in finite incommensurate contacts. The effects of sliding velocity, flake size, and amplitude of substrate potential corrugation on the frictional energy dissipation were studied. Different dynamical regimes of friction as a function of internal and external parameters of the system are investigated. The results obtained can be used for estimations of edge contribution² to overall friction in incommensurate macroscale contacts and for rational design of superlubric contacts.

References:

1. Norell, J.; Fasolino, A.; de Wijn, A. S. Emergent Friction in Two-Dimensional Frenkel-Kontorova Models. *Phys. Rev. E* **2016**, *94* (2), 023001.
2. Wang, J.; Cao, W.; Song, Y.; Qu, C.; Zheng, Q.; Ma, M. Generalized Scaling Law of Structural Superlubricity. *Nano Lett.* **2019**, *19* (11), 7735-7741.

Djoumekam Mouafo Laure

Title: Anisotropie de friction des structures de bisulfure de molybdène et du graphite à l'échelle nanométrique

Abstract: L'object de notre travail est d'étudié L'anisotropie comport

de friction suivant toutes les directions sur les surfaces du bisulfure de molybdène et du graphite à l'échelle nanométrique avec le modèle de Prandtl-Tomlinson en considérant l'influence de la température et du paramètre de déformabilité.

Nous obtenons deux symétries à savoir : la symétrie double et la symétrie sextuple.

Suivant les directions de symétrie double pour la surface du bisulfure de molybdène, l'amplitude de la force de friction est plus grand par rapport à celle des directions sextuple. Pour la surface du graphite l'amplitude de la force de friction est très faible suivant les directions de symétrie double. Avec l'augmentation du paramètre de déformabilité nous obtenons le régime de super lubrification.

Self-organization of horizontally agitated microspheres

Ignas S.M. Jimidar^{1,2}, Kai Sotthewes³, Han Gardeniers², Gert Desmet¹, and Devaraj van der Meer⁴

¹ Department of Chemical Engineering, Vrije Universiteit Brussel, Belgium

² Mesoscale Chemical Systems group, University of Twente, The Netherlands

³ Physics of Interfaces and Nanomaterials group, University of Twente, The Netherlands

⁴ Physics of Fluids group, University of Twente, The Netherlands.

The vibration dynamics of relatively large granular grains is extensively treated in literature, but comparable studies on the self-assembly of smaller agitated beads are lacking. In this work, we investigate how the particle properties and the properties of the underlying substrate surface affect the dynamics and self-organization of horizontally agitated monodisperse microspheres with diameters between 3 and 10 μm (cf. Fig. 1a).[1] Upon agitation, the agglomerated hydrophilic silica particles locally leave traces of particle monolayers as they move across the flat uncoated and fluorocarbon-coated silicon substrates. However, on the micromachined silicon tray with relatively large surface roughness, the agitated silica agglomerates form segregated bands reminiscent of earlier studies on granular suspensions or Faraday heaps (cf. Fig. 1b). The formed monolayers are inspected with a scanning electron microscope (SEM) and their symmetry is studied using Voronoi analysis (cf. Fig. 1c). Using Kelvin probe force microscopy measurements, we show that due to the tribocharging phenomenon, the formation of particle monolayers is promoted on the fluorocarbon surface (cf. Fig. 1d).

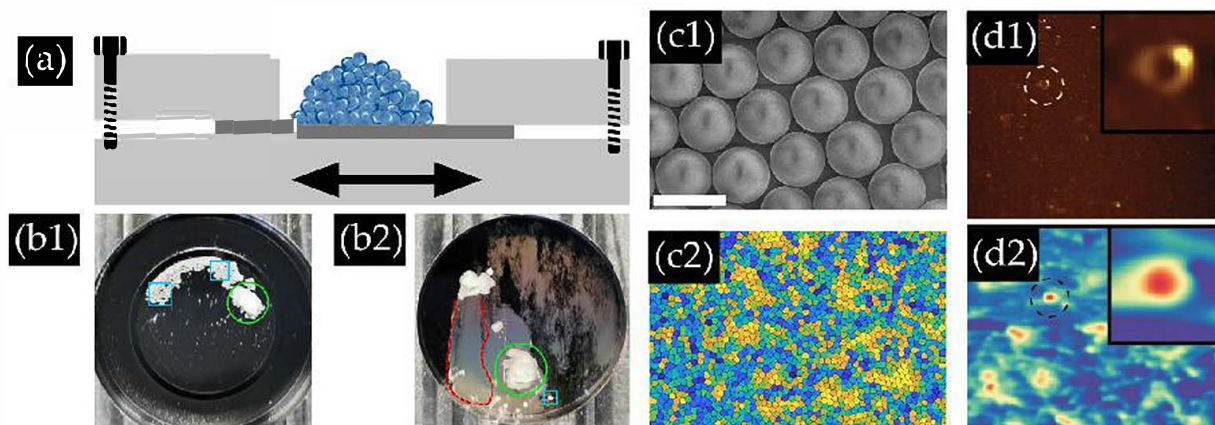


Figure 1: (a) Schematic representation of the experiment in which microspheres are agitated laterally on various substrates. The global distribution of 10 μm silica microspheres on (b1) an etched silicon particle tray and (b2) a fluorocarbon-coated silicon substrate. (c1) The microscopic distribution of the 10 μm polystyrene microspheres and (c2) the corresponding Voronoi diagram of the assembled monolayer on a fluorocarbon-coated substrate. (d1) The topography and (d2) and corresponding surface potential map of the fluorocarbon-coated substrate performed with the Kelvin probe force microscope after the agitation experiment with silica particles. Scale bar is 10 μm , green circles represent the large luster, blue squares represents smaller silica clusters, and red dashed lines represent the formed monolayers.

[1] I.S.M. Jimidar, K. Sotthewes, H. Gardeniers, G. Desmet, D. van der Meer, *Soft Matter* **18**, 3660 - 3677 (2022).

Ripple formation and evolution in compliant materials

Juan J. Mazo¹, Pedro J. Martínez², and Enrico Gnecco³

¹*Universidad Complutense de Madrid, 28040 Madrid, Spain*

²*Instituto de Nanociencia y Materiales de Aragón, CSIC-Universidad de Zaragoza, and Universidad de Zaragoza, 50009 Zaragoza, Spain*

³*Marian Smoluchowski Institute of Physics, Jagiellonian University, 30-348 Krakow, Poland*

In 1992 Leung and Goh [1] published a pioneering work in which they showed the ability of an AFM tip to generate a series of wavy patterns (usually known today as ripples) when scanning a polymer surface. There, the effect of the AFM is to mold the surface itself, which deforms under the pressure exerted by the tip. Leung and Goh's work opened an important experimental line in the field, which has led to remarkable advances. However, a theoretical approach to the underlying basic mechanisms under this effect has been elusive for many years.

Starting from previous works, we have developed a model that has allowed to study numerically in 3d the problem [2]. The theoretical approach used starts from the observation of the stick-slip phenomenon in the experiments and is built from the basic premises of the Prandtl-Tomlinson model: a point object that interacts with the support and the surface. But its great novelty is that the tip-substrate interaction potential changes over time under the action of the tip. That is, the model combines the plastic deformation of the surface with the elastic deformation of the AFM tip, proposing a system of equations for the motion of the tip interacting with a surface potential that also changes in time under the action of a point moved by a support at a certain speed.

Based on this model, we have managed to reproduce various characteristics of the patterns found experimentally, obtaining both a quantitative and qualitative agreement between our simulations and the main experimental observations [2, 3, 4, 5].

- [1] O.M. Leung, M. C. Goh, Orientational ordering of polymers by atomic force microscope tip-surface interaction. *Science* 255, 64 (1992).
- [2] J. J. Mazo, P. J. Martínez, P. Pedraz, J. Hennig, and E. Gnecco, Plowing-Induced Structuring of Compliant Surfaces. *Phys. Rev. Lett.* 122, 256101 (2019).
- [3] J. Hennig, A. Litschko, J. J. Mazo, E. Gnecco, Nucleation and detachment of polystyrene nanoparticles from plowing-induced surface wrinkling. *App. Surf. Sci. Adv.* 6, 100148 (2021).
- [4] P. J. Martínez, E. Gnecco, and J. J. Mazo, Numerical study of pattern formation in compliant surfaces scraped by a rigid tip. *Phys. Rev. E* 103, 022802 (2021).
- [5] J. Hennig, V. Feller, P. J. Martínez, J. J. Mazo, and E. Gnecco, Locking effects in plowing-induced nanorippling of polystyrene surfaces. *App. Surf. Sci.* (to appear).

Tribological study of Fe-Based Amorphous Nanocomposite Coatings Reinforced by B₄C Nanoparticles

Behrooz Movahedi¹

¹ *Department of Nanotechnology, Faculty of Chemistry, University of Isfahan, Isfahan, 81746-73441, Iran*

The feedstock nanocomposite powders of Fe-based amorphous matrix with various ratios of hard B₄C nanoparticles were transferred to the coatings using a high-velocity oxygen fuel (HVOF) process. The results showed that the microstructure of the nanocomposite coating was divided into two regions, namely a full amorphous phase region and homogeneous dispersion of B₄C nanoparticles. As the B₄C content is increased, the hardness of the composite coatings is increased too, but the fracture toughness begins to be decreased. The optimal tribological properties are obtained with 15 vol pct B₄C due to the reduced the friction coefficient from 0.49 to 0.28. The average specific wear rate of the nanocomposite coating ($0.48 \times 10^{-5} \text{ mm}^3 \text{ Nm}^{-1}$) was much less than that for the single-phase amorphous coating ($1.23 \times 10^{-5} \text{ mm}^3 \text{ Nm}^{-1}$). Consequently, the changes in wear resistance between both coatings were attributed to the changes in the brittle to ductile transition by adding B₄C reinforcing nanoparticles.

Speaker: MUGWANEZA Denyse, Rwanda Mines, Petroleum and Gas Board

DEVELOPMENT OF ACTIVATED CARBON FROM WASTE

Activated Carbon (AC) has extended its use in the past years due to the uniqueness of physical properties at nanoscale levels and adsorption properties as well. It is carbonized material having high porosity and wide surface area and thus its application in Energy storage and environmental remediation for removing, separating, and modifying different compounds from aqueous media is appreciated. Activated Carbon is applied in various environmental applications ranging from water and wastewater treatments, gas filtration, and natural gas storage and among others. Scientists are working hard to use green technology and science to promote environmental protection. The term green technology is used to describe innovative solution to create and conserve environmental in sustainable way. The green technology is applied to reduce waste and environmental pollution associated with production and consumption of resources. The carbon containing waste will be collected and unit operation will be developed to transform waste into activated carbon. SEM analysis will be done to evaluate the efficacy of developed activated carbon.

Magnetic spin losses, Competing Interactions, and magnetization dynamics in Doped Rare-earth Manganites nanostructural system

Wiqar Hussain Shah,
Department of Physics, Faculty of Basic and Applied Sciences,
Islamic International University, Islamabad, Pakistan

Abstract:

The Structural, magnetic and transport behavior of $\text{La}_{1-x}\text{Ca}_x\text{MnO}_{3+\delta}$ ($x=0.48, 0.50, 0.52$ and 0.55 and $\delta=0.015$) compositions close to charge ordering, was studied through XRD, resistivity, DC magnetization and AC susceptibility measurements. With time and thermal cycling ($T < 300$ K) there is an irreversible transformation of the low-temperature phase from a partially ferromagnetic and metallic to one that is less ferromagnetic and highly resistive. For instance, an increase of resistivity can be observed by thermal cycling, where no effect is obtained for lower Ca concentration. The time changes in the magnetization are logarithmic in general and activation energies are consistent with those expected for electron transfer between Mn ions. The data suggest that oxygen non-stoichiometry results in mechanical strains in this two-phase system, leading to the development of irreversible metastable states, which relax towards the more stable charge-ordered and antiferromagnetic microdomains at the nano-meter size. This behavior is interpreted in terms of strains induced charge localization at the interface between FM/AFM domains in the antiferromagnetic matrix. Charge, orbital ordering and phase separation play a prominent role in the appearance of such properties, since they can be modified in a spectacular manner by external factor, making the different physical properties metastable. Here we describe two factors that deeply modify those properties, viz. the doping concentration and the thermal cycling. The metastable state is recovered by the high temperature annealing. We also measure the magnetic relaxation in the metastable state and also the revival of the metastable state (in a relaxed sample) due to high temperature (800 C°) thermal treatment.

Effect of entropy changes on time to failure caused by tribological causes

V. V. Ryazanov

Institute for Nuclear Research, Kiev, Ukraine, e-mail: vryazan19@gmail.com

In works [1-3], the first passage time (FPT) is associated with the entropy changes in the system that occur during this time. The impact of entropy changes on the mean FPT can be significant [4]. Such estimates can be made for the time until the failure of some node of the system or until the end of some stage of the operation process. Data on entropy changes are taken from tribological studies. The key issue is the choice of distribution for the FPT. One of the possible solutions can be the maximum entropy method with restrictions corresponding to the specifics of the process. This approach makes it possible to isolate the contributions from various processes (friction, wear, structural-phase transformations, physico-chemical processes, etc.), evaluate them, and choose the optimal ways of influencing the system.

1. V. V. Ryazanov, First passage time and change of entropy, *Eur. Phys. J. B*, **94**, 242 (2021). <https://doi.org/10.140/epjb/s10051-021-00246-0>.
2. V. V. Ryazanov, S. G. Shpyrko, First-passage time: a conception leading to superstatistics. *Condensed Matter Physics*, **9**, 1(45), 71-80 (2006).
3. V. V. Ryazanov, Lifetime distributions in the methods of non-equilibrium statistical operator and superstatistics, *European Physical Journal B*, **72**, 629–639, (2009).
4. 8. V. V. Ryazanov, First passage times of mesoscopic charge transport and entropy change. <https://arxiv.org/abs/2201.06497>.

Magnetic spin losses, Competing Interactions, and magnetization dynamics in Doped Rare-earth Manganites nanostructural system

Wiqar Hussain Shah,
Department of Physics, Faculty of Basic and Applied Sciences,
Islamic International University, Islamabad, Pakistan

Abstract:

The Structural, magnetic and transport behavior of $\text{La}_{1-x}\text{Ca}_x\text{Mn}_{3+\delta}$ ($x=0.48, 0.50, 0.52$ and 0.55 and $\delta=0.015$) compositions close to charge ordering, was studied through XRD, resistivity, DC magnetization and AC susceptibility measurements. With time and thermal cycling ($T < 300$ K) there is an irreversible transformation of the low-temperature phase from a partially ferromagnetic and metallic to one that is less ferromagnetic and highly resistive. For instance, an increase of resistivity can be observed by thermal cycling, where no effect is obtained for lower Ca concentration. The time changes in the magnetization are logarithmic in general and activation energies are consistent with those expected for electron transfer between Mn ions. The data suggest that oxygen non-stoichiometry results in mechanical strains in this two-phase system, leading to the development of irreversible metastable states, which relax towards the more stable charge-ordered and antiferromagnetic microdomains at the nano-meter size. This behavior is interpreted in terms of strains induced charge localization at the interface between FM/AFM domains in the antiferromagnetic matrix. Charge, orbital ordering and phase separation play a prominent role in the appearance of such properties, since they can be modified in a spectacular manner by external factor, making the different physical properties metastable. Here we describe two factors that deeply modify those properties, viz. the doping concentration and the thermal cycling. The metastable state is recovered by the high temperature annealing. We also measure the magnetic relaxation in the metastable state and also the revival of the metastable state (in a relaxed sample) due to high temperature (800 C°) thermal treatment.



Frictional dissipation in the 2D Prandtl-Tomlinson model

M. Srbulovic¹, K. Gkagkas², and A. Vernes^{1,3}

¹AC2T research GmbH, Wiener Neustadt, Austria

²Material Engineering Division, Toyota Motor Europe NV/SA, Zaventem, Belgium

³Institute of Applied Physics, TU Wien, Vienna, Austria

Prandtl-Tomlinson models (PT-models) in one or two dimensions (2D) are widely considered for explaining nanotribological experiments when these are performed by using a friction or atomic force microscope (AFM) [1]. In its original formulation [2], Prandtl was introducing this model while elaborating a kinetic theory of solids assuming a periodic interaction between the bodies. Curiously, in the other historical paper ascribed to the PT-models [3], Tomlinson was establishing a molecular theory of friction based on the Lennard-Jones potential.

A numerical scheme was recently developed by the authors [4], for a statistically proper comparison of the frictional performance obtained by applying the 2D PT-model for describing the sliding on (a)periodic atomic structures and within various regimes, e.g., stick-slip or superlubric. This was motivated by the thermally induced random force entering the Newtonian equations of motion, which so are forming a set of stochastic differential equations within the 2D PT-model. This random force mimicking the impact of temperature on sliding, makes it necessary to statistically analyze and interpret, for example, in terms of distributions, the numerically determined frictional and reaction forces.

Beyond this, the same statistical scheme will be applied here for also studying the work done by both frictional and reaction forces acting on an AFM-tip towards to obtain statistically proper insights on the dissipation in various sliding regimes, see Fig. 1.

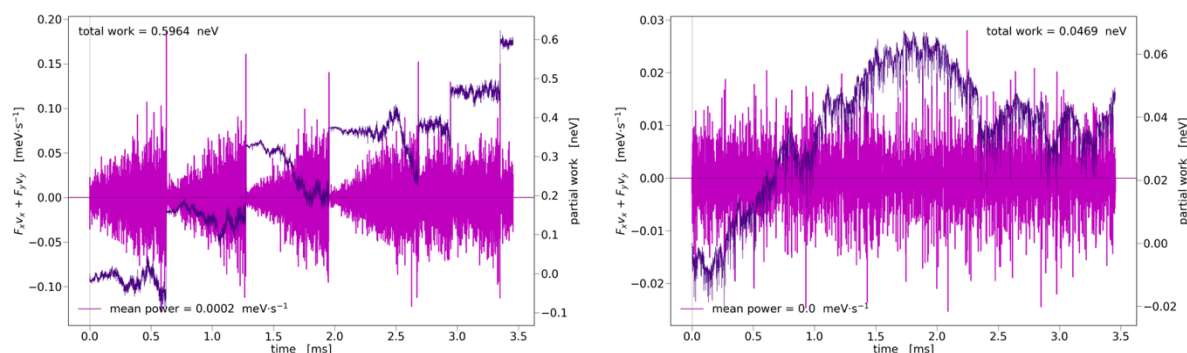


Fig.1: Time-resolved power and work done by an AFM-tip within a stick-slip (left) and superlubric (right) sliding regime .

This work was funded by the Austrian COMET-Program (project K2 InTribology1, no. 872176). The work has been carried out within the “Excellence Centre of Tribology” (AC2T research GmbH).

[1] U. D. Schwarz, H. Hölscher, ACS Nano **10**, 38 (2016).

[2] L. Prandtl, Z. Angew. Math. Mech. **8**, 85 (1928).

[3] G. A. Tomlinson, Philos. Mag. **7**, 905 (1929).

[4] M. Srbulovic, K. Gkagkas, C. Gachot, A. Vernes, Frontiers in Mech. Eng. **7**, 742684 (2021).