

# 2D Materials for Super-Low Friction Coatings (Ramot)

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#### Technology

Solid super lubricant coatings based on heterogeneous structures, composed of several layered materials. Theses permanent surface coatings are expected to result in robust ultra-low friction characteristics at different scales ranging from the nanoscale up to the macro scale. The technology sets the ground for a new generation of low-energy consumption and highly durable mechanical devices with an expected global impact.

## The Need

Friction is one of the oldest and continuously active research areas in science and technology. It is estimated that about 1/3 of the global energy dissipation in developed countries is caused by friction; 80% of mechanical failure of machine parts is caused by wear, which leads to a loss of about 5%-7% of the GDP in industrial countries. Using materials that present super-low friction (superlurbricity) may provide a desired route to overcome these major problems.

## **Potential Application**

The diverse potential applications of such materials include information storage devices, high precision positioning systems, mobile frictionless connectors, medicinal products such as automatic syringes, micro-electro-mechanical systems, and lubrication in extreme temperature and pressure conditions such as those appearing at nanoscale constrictions and space applications.

# **Stage of Development**

Over the past few years many computational studies have focused on understanding the friction properties of nanoscale junctions. Several approaches range from highly accurate ab-initio characterizations of miniature junction models, through fully atomistic simulations of junction friction and ware, molecular dynamics simulations of phenomenological junction models, and geometrical characterization of large-scale material junctions.

While atomistic representations of interfaces often provide good agreement with experiments, their application is limited to relatively small dimensions and short time scales. Furthermore, their complexity may make it hard to identify and isolate the important physical parameters underlying the tribological processes under study. Phenomenological and geometric models, on the other hand, may provide important general insights on the frictional properties of material interfaces and can elucidate the main factors that dictate their tribological characteristics.

The joint expertise of the groups of Prof. Urbakh and Prof. Hod range from the development of fully atomistic force fields to describe the interlayer interactions in heterogeneous layered junctions, through large-scale molecular dynamic simulations based on specifically design phenomenological Hamiltonians, to the development of geometric models to characterize the sliding energy landscape in large-scale material junctions.

At present, they are actively working on the development of dedicated force fields that provide reliable description of the interlayer interactions in a variety of layered materials including graphene, hexagonal boron nitride, and heterojunctions thereof. Furthermore, we are working on molecular dynamics simulations of the friction and ware in metal surfaces coated by graphene in a wide range of normal-loads and velocities. In addition, their recently developed registry index method is currently fully developed to be used in the suggested scenarios. All these available method allow them to cover a large spectrum of scales ranging from the nanoscale up to the macroscopic world and propose rationally designed new heterogeneous structures presenting desired frictional properties.

On the experimental side, Dr. Ismach has been working during the past several years on the developing of methodologies for the controlled growth of graphene, hexagonal boron nitride (h-BN) and transition metal dichalcogenides (mainly MoS2 and WSe2). He has proven track in the synthesis

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of single- and few-layer graphene and h-BN. He has extensive experience in the synthesis and characterization of single- and few-layer graphene by surface-mediated growth (i.e. on copper) or by diffusion and segregation from the bulk (on nickel, cobalt, etc.). That includes the transfer of the atomic-films to the target substrate for characterization and device processing. In the case of h-BN, he has shown the possibility to control the thickness of a high quality h-BN ultra-thin film from ~1-3 layers to ~100 layers by monitoring the growth conditions. The synthesis of large scale h-BN single-crystal and single-layer of ~100 �m was also demonstrated. Furthermore, he has gainedsignificant experience on the challenging characterization of atomic-films heterostructures by Raman spectroscopy, x-ray photoelectron spectroscopy (XPS) and time-of-flight secondary ion mass spectroscopy (TOF-SIMS). All this work was published in the last several years. Dr. Ismach's expertise in the challenging synthesis and characterization of 2D materials in general will play a key role in the assembly of 2D material heterostructures for friction measurements.

# Patents

A provisional patent application is being filed

# **Supporting Publications**

I. Leven, I. Azuri, L. Kronik, and O. Hod, "Inter-Layer Potential for Hexagonal Boron Nitride", J. Chem. Phys. 140, 104106 (2014).

O. Y. Fajardo, F. Bresme, A. Kornyshev and M. Urbakh, "Electrotunable Lubricity with Ionic Liquid Nanoscale Films", Scientific Reports 5, 7698 (2015).

O. Hod, "The Registry Index: A Quantitative Measure of Materials Interfacial Commensurability", ChemPhysChem 14, 2376-2391 (2013).

A. Ismach, C. Druzgalski, S. Penwell, M. Zheng, A. Javey, J. Bokor, and Y. Zhang, "Direct Chemical Vapor Deposition of Graphene on Dielectric Surfaces", Nano Letters 10, 1542-1548 (2010)

A. Ismach, H. Chou, D. Ferrer, Y. Wu, H.C. Floresca, S. McDonnell, A. Covacevich, C. Pope, R. Piner, R. Wallace, M. Kim, L. Colombo, and R. Ruoff, "Towards the Controlled Synthesis of hexagonal Boron Nitride Films" ACS Nano 6, 6378–6385 (2012)

Y. Liu, R. Ghosh, D. Wu, A. Ismach, R.S. Ruoff, and K. Lai "Mesoscale Imperfections in MoS2 Atomic Layers Grown by Vapor Transport Technique" Nano Letters, 14, 4682-4686 (2014)

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