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Modeling Interlayer Interactions in Layered Materials

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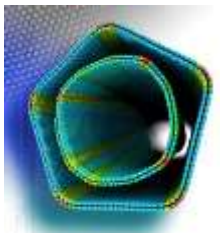
Abstract:



In the past two decades low dimensional layered nano-materials have been at the forefront of scientific research. Owing to a variety of novel outstanding physical properties graphene, hexagonal boron nitride (*h*-BN), and transition metal dichalcogenides (TMDC) hold great promise for becoming key components in the next generation of advanced electronics, strong lightweight materials, and friction reducing technologies. The interlayer interactions in these materials play a central role in shaping their mechanical and electronic properties.

In my lecture, I will present a new methodology for modeling these interactions using specially tailored classical force-fields. The computational capabilities of the developed methodology will be demonstrated via several applications addressing the structural, mechanical, and tribological properties of layered materials including the super-structure of the graphene/*h*-BN heterojunction, which has been shown to alter graphene's electronic properties, the occurrence of robust structural superlubricity and negative friction coefficients in heterojunctions of layered materials, the motion of nanoserpents, the occurrence of circumferential faceting in double-walled nanotubes, motion over grain boundaries, and penetration of surface perturbations into the anisotropic bulk material. Then I will turn to describe interlayer electrical conductance across a twisted graphene interface, where I will show the strong correlation between interlayer structural commensurability and cross-layer electrical transport.

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Date & Location:

Tuesday, June 9, 2020, 11:00
Lecture room, Physics Building (ground floor)

1. W. Ouyang, I. Azuri, D. Mandelli, A. Tkatchenko, L. Kronik, M. Urbakh, and O. Hod, "Mechanical and Tribological Properties of Layered Materials Under High Pressure: Assessing the Importance of Many-Body Dispersion Effects", *J. Chem. Theory Comput.*, in press (2019).
2. D. Mandelli, W. Ouyang, M. Urbakh, and O. Hod, "The Princess and the Nanoscale Pea: Long-Range Penetration of Surface Distortions into Layered Materials Stacks", *ACS Nano* **13**, 7603-7609 (2019).
3. D. Mandelli, W. Ouyang, O. Hod, and M. Urbakh, "Negative Friction Coefficient in Superlubric Graphite/Hexagonal Boron Nitride Heterojunctions", *Phys. Rev. Lett.* **122**, 076102 (2019).
4. O. Hod, E. Meyer, Q. Zheng, and M. Urbakh, "Structural Superlubricity and Ultralow Friction Across the Length Scales", *Nature* **563**, 485-492 (2018).
5. Y. Song, D. Mandelli, O. Hod, M. Urbakh, M. Ma, and Q. Zheng, "Robust Microscale Superlubricity in Graphite/Hexagonal Boron Nitride Layered Heterojunctions", *Nat. Mater.* **17**, 894-899 (2018).
6. W. Ouyang, D. Mandelli, M. Urbakh, and O. Hod, "Nanoserpents: Graphene Nanoribbon Motion on Two-Dimensional Hexagonal Materials", *Nano Lett.* **18**, 6009-6016 (2018).
7. T. Maaravi, I. Leven, I. Azuri, L. Kronik, and O. Hod, "Interlayer Potential for Homogeneous Graphene and Hexagonal Boron Nitride Systems: Reparameterization for Many-Body Dispersion Effects", *J. Phys. Chem. C* **121**, 22826-22835 (2017).
8. R. Guerra, I. Leven, A. Vanossi, O. Hod, and E. Tosatti, "Smallest Archimedean Screw: Facet Dynamics and Friction in Multi-Walled Nanotubes", *Nano Lett.* **17**, 5321-5328 (2017).
9. D. Mandelli, I. Leven, O. Hod, and M. Urbakh, "Sliding Friction of Graphene/Hexagonal-Boron Nitride Heterojunctions: A Route to Robust Superlubricity", *Sci. Rep.* **7**, 10851 (2017).
10. I. Leven, T. Maaravi, I. Azuri, L. Kronik, and O. Hod, "Inter-Layer Potential for Graphene/*h*-BN Heterostructures", *J. Chem. Theory Comput.* **12**, 2896-2905 (2016).
11. Faceting. Unravelled", *Nat. Nanotechnol.* **11**, 1082-1086 (2016).
12. E. Koren, I. Leven, E. Lörtscher, A. Knoll, O. Hod, and U. Duerig, "Coherent Commensurate Electronic States at the Interface Between Misoriented Graphene Layers", *Nat. Nanotechnol.* **11**, 752-757 (2016).
13. [I. Leven, I. Azuri, L. Kronik, and O. Hod, "Inter-Layer Potential for Hexagonal Boron Nitride", *J. Chem. Phys.* **140**, 104106 (2014).
14. O. Hod, "The Registry Index: A Quantitative Measure of Materials Interfacial Commensurability", *ChemPhysChem* **14**, 2376-2391 (2013).
15. I. Leven, D. Krepel, O. Shemesh, and O. Hod, "Robust Superlubricity in Graphene/*h*-BN Heterojunctions", *J. Phys. Chem. Lett.* **4**, 115-120 (2013).