



The Hebrew University Center
for Nanoscience & Nanotechnology



Nano Seminar

Modeling Interlayer Interactions in Layered Materials

Prof. Oded Hod

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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 graphene/*h*-BN heterojunction, which has been shown to alter graphene electronic properties, and the occurrence of circumferential faceting in double-walled nanotubes. 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.

Gathering & Refreshments at 10:50

Please contact Alexandra Bannykh at 6584919 if you are interested in meeting the lecturer.

Tuesday, Mar 14th 2017, 11:00 at the Seminar Hall

Los Angeles Building, entrance floor.