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S E M I N A R
on
Semiconductor Physics and Nanotechnology

Mo, 13.11.2023, 11:15 Uhr,

Seminar in person in the Physics lecture hall *or* via Zoom

"Exploring Collective Dynamics of Small Molecules on Carbon-Based Layered Materials with Molecular Dynamics Simulations"

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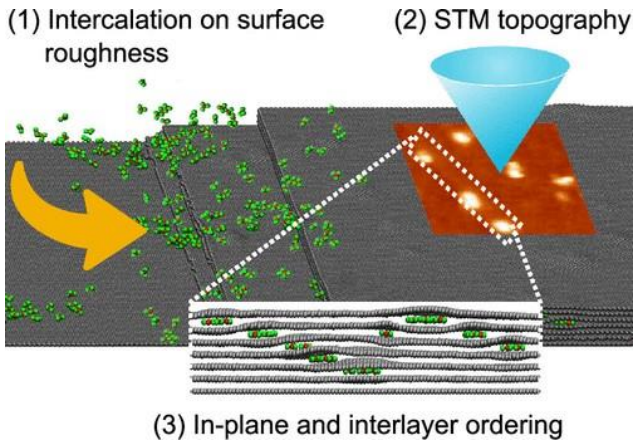
This presentation delves into the intriguing world of small molecules and their collective dynamics, offering insights into their behavior in diverse nanoscale systems. Graphite and graphene, are two remarkable carbon-based materials, that have been at the forefront of a revolution in the fields of energy storage and two-dimensional electronics. Graphite, a layered material composed of stacked graphene sheets, has long been used as the anode material in conventional lithium-ion batteries. However, the quest for higher energy density and faster charging capabilities has driven researchers to explore novel electrolytes and modifications of graphite. Graphene, the single-layer counterpart of graphite, comprises a honeycomb lattice of carbon atoms. Graphene is incredibly thin, lightweight, and possesses outstanding electrical conductivity. This talk presents three examples where molecular dynamics simulations were combined with state-of-the-art experiments to reveal the fascinating diversity of collective interactions of small molecules in contact with carbon-based layered materials.

At the largest scale, we challenge conventional paradigms by investigating friction mechanisms in hydrophobic contact with highly ordered pyrolytic graphite HOPG [1]. Through a combination of experimental investigations and molecular dynamic simulations, we introduce a novel mechanism involving the agglomeration dynamics of water droplets, resulting in the formation of larger droplets within sliding nano-contacts. This mechanism elucidates the experimental tribological behavior, emphasizing the crucial role of water molecules in understanding friction on hydrophobic surfaces.

The second study focuses on the intercalation mechanism of aluminum fluoride (AlF3), a small molecule, into graphite electrodes in rechargeable aluminum batteries [2]. By employing scanning tunneling microscopy, density functional theory calculations, and large-scale molecular dynamics simulations, we unravel the collective dynamics of AlF3 clusters between graphite layers. This knowledge enhances our understanding of the mobility and clustering of small molecules within anode materials, paving the way for performance enhancements in energy storage systems.

In previous examples, we saw how large electric dipole moments of molecules influence the mechanical and functional properties of graphite. In the final part of the talk, we demonstrate how

molecular dynamics simulations can reproduce geometry and conditions close to experimental [3]. The interaction mechanism of including the collective motion of water molecules within clusters under varying external electric fields is uncovered with a particular focus on molecular ferroelectric devices anchored to bilayer graphene nanoribbons. Combining experiments with large-scale molecular dynamics simulations, we unveil the behavior of these small water clusters, emphasizing their role in generating ferroelectric effects and persistent remanent fields for potential applications in ferroelectric heterostructures and neuromorphic circuits.



Zoom – Link:
https://zoom.us/j/96375934537?pwd=RTlKTWhSdzRHU211YTY1bGFxTUtpZz09
Meeting-ID: 963 7593 4537
Kenncode: =r=4YQ

[1] M.A. Aslam, I. Stankovic, G. Murastov, A. Carl, Z. Song, K. Watanabe, T. Taniguchi, A. Lugstein, C. Teichert, R. Gorbachev, R. D. Rodriguez, and A. Matkovic, Water Induced Ferroelectric Switching: The Crucial Role of Collective Dynamics, submitted to Nano Letters, arXiv preprint arXiv:2304.09738.
[2] S.J. Rodríguez, A.E. Candia, I. Stanković, M.C.G. Passeggi, and G.D. Ruano, Study of in-plane and interlayer interactions during aluminum fluoride intercalation in graphite: implications for the development of rechargeable batteries, ACS Applied Nano Materials, 6 (18), 16977–16985 (2023).
[3] O. Noël, P.E. Mazeran, and I Stankovic Nature of dynamic friction in a humid hydrophobic nanocontact, ACS Nano 16 (7), 10768-10774 (2022).