Computational Methodologies for Unraveling Dynamics in Bio-nanoscale Devices

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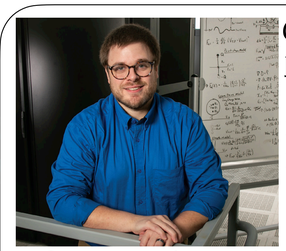
JSNN Joint School of Nanoscience and Nanoengineering



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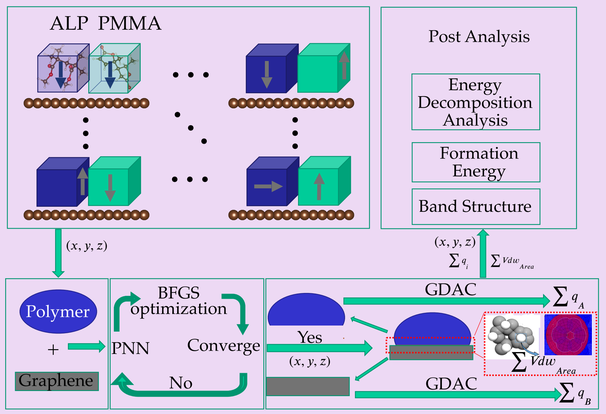
Computational material science is analogous to computational biology or computational physics. It utilizes modeling, simulation and theory to discover new materials and determining behavior and mechanisms.

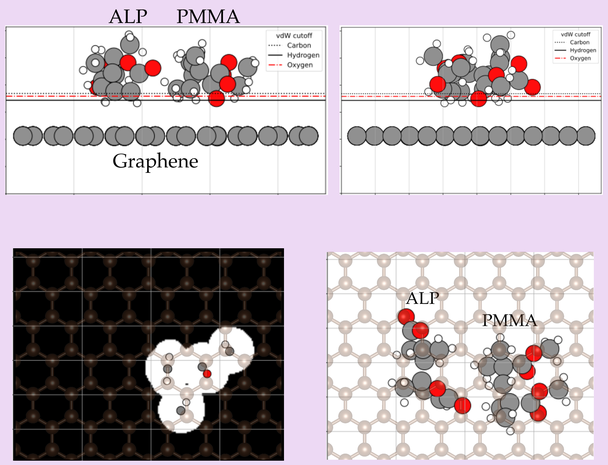
Generalized High-Throughput Method for Nano-device discovery

Jared Keith Averitt, Joseph Starobin, Tetyana Ignatova

High-Throughput / PNN



vdW-overlap E-correction

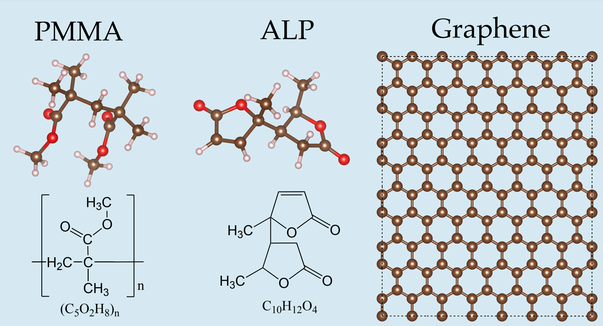


Nano-bio interactions are computationally challenging. We used a neural network approach, bypassing time-related issues in electron configurations like DFT simulations. This method explores various configurations efficiently, enabling probabilistic approaches by investigating millions of relaxed energy geometries in nano-bio interactions.

Clean Transfer of CVD Graphene via Biomass-derived Polymer Mixture: Neural Network Simulations

Jared Keith Averitt, Sajedeh Pourianejad, Olubunmi Ayodele, Kirby Schmidt, Anthony Trofe, Joseph Starobin, Tetyana Ignatova

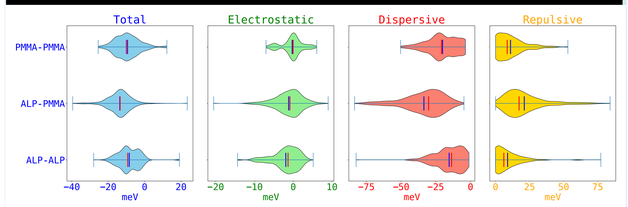
Polymer & Graphene Systems



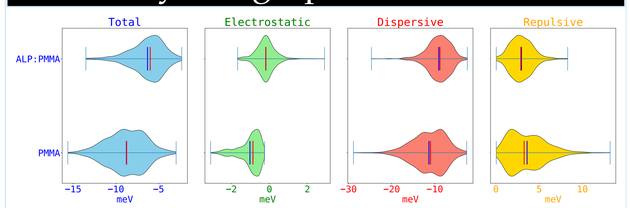
Energy Decomposition Analysis

$$E_{tot} = \frac{q_A q_B}{r_{AB}} + \varepsilon_{AB}\left(\frac{R^0_{AB}}{r_{AB}}\right)^{12} - 2\varepsilon_{AB}\left(\frac{R^0_{AB}}{r_{AB}}\right)^{6}$$

Polymer-polymer Results



Polymer-graphene Results

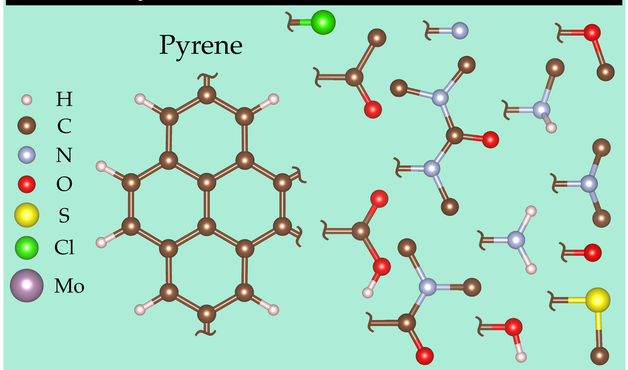


This study quantified the fundamental forces between two polymers interacting with graphene during device fabrication procedure. Mixing them results in cleaner graphene devices. Simulations showed a substantial decrease in interaction energy and electrostatic interaction between the polymers. The aim is to increase the use of biomass-derived polymers like ALP in device fabrication for environmental sustainability (and biodegradable).

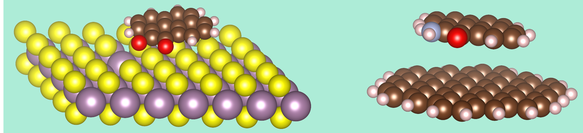
Neural Network Method for the Discovery of Sensors to Detect Amine Compounds

Jared Keith Averitt, Isaiah Moses, Boyang Zheng, Vincent Crespi, Wesley Reihnhart, Micheal Ghebrebrham, Joseph Starobin, Tetyana Ignatova

Pyrene Functionalization



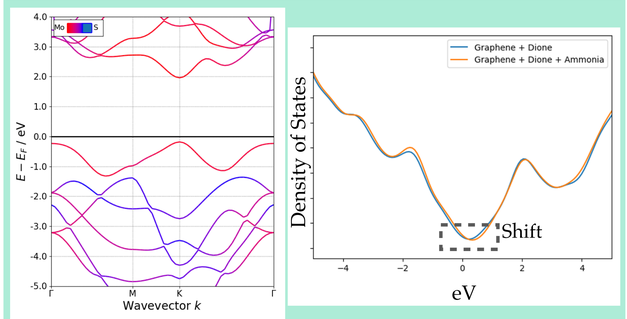
2DM Sensors



4,5-pyrene-dione on a MoS_2 layer with S vacancy

4-one,5-imine-pyrene on a graphene flake

Results

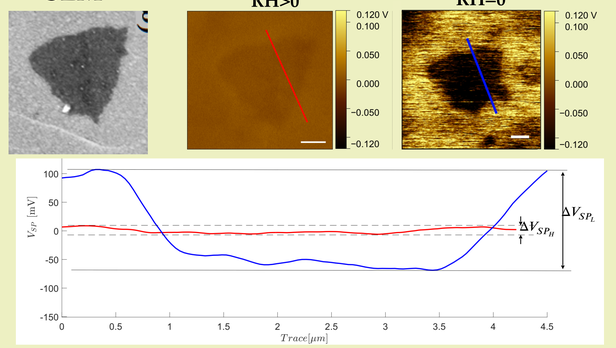


Simulations can guide experiments, optimizing time. Initially, we screen sensors for notable changes, like band structure shifts post-bioanalyte exposure. Later, a smaller sensor group undergoes testing to measure effectiveness. These sensors primarily target detecting low concentrations of ammonia in urea samples such as from blood in diabetic patients.

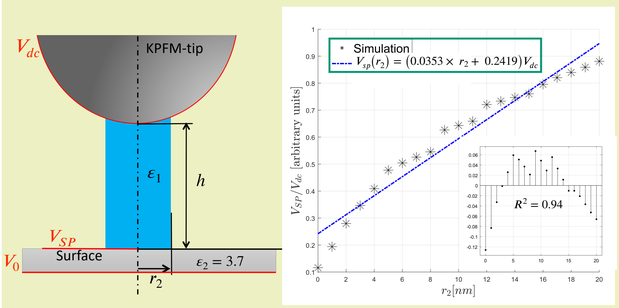
Deconvolution of the Electric-shielding Effect of Ubiquitous Water in Kelvin Probe Force Microscopy

Jared Keith Averitt, Anthony Trofe, Sajedeh Pourianejad, Joseph Starobin, Tetyana Ignatova

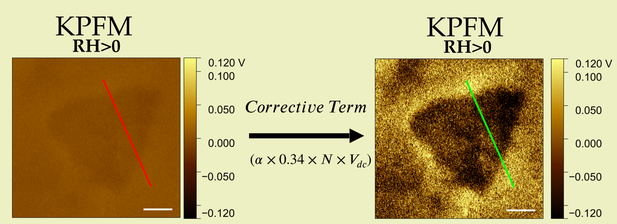
Experimental Observations



FE Simulation / Fitted Model



Results



Biological systems rely on surface potentials and electrostatic interactions for cellular functions like cardiac activity, ion channels, and protein behavior. To understand this, we studied a heterostructure using KPFM at varying humidity levels. Using a Finite Element model and Maxwells Equation, we delved into how water affects surface potential difference between a simulated tip and a non-metallic surface.

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Professor Reinhart, Dr. Moses

Members of Tetyana Ignatova's Lab

Dr. Sajedeh, Professor Tetyana Ignatova, Dr. Kirby, Dr. Olubunmi, Anthony Trofe

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