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Development and Validation of Polarized Models for Peptide-Graphene Interactions HENDRIK HEINZ, AMANDA GARLEY, NABANITA SAIKIA, University of Colorado - Boulder, STEPHEN BARR, GARY LEUTY, RAJIV BERRY, Air Force Research Laboratory — Biosensor technologies require the understanding of interactions between organic and inorganic materials to tune electric response functions, such as peptide assembly on graphitic substrates. Laboratory characterization of specific interactions and molecular assembly of such biomolecules in atomic resolution remains challenging. These methods can be complemented by molecular simulations and quantum-mechanical analysis of band gaps and expected conductivity. We improved common dispersive interatomic potentials for graphite and graphene to include pi electron density at virtual sites. The new models reproduce experimental X-ray structure, density, cleavage energy, hydration energy, and contact angles. As a result we have improved existing models which gave the wrong sign of hydration energies and deviations on the order of 30% in other properties. The parameters are embedded in CHARMM, CVFF, TEAM-AMBER, and other common force fields as part of the INTERFACE force field. An analysis of binding residues, binding energies, conformations, and dynamic information of molecular mobility on the surfaces will be presented.

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