Surface-Dependence of Interfacial Binding Strength between Zinc Oxide and Graphene Investigated from First Principles

Allyse Appel, Adam Clark, Kelsey Larson, Haiying He, Stan Zygmunt

Departmental Affiliation: Physics and Astronomy
College of Arts and Sciences

There is an increasing interest in hybridized materials for applications such as improving the structural integrity of known and commonly used materials. Recent experiments have suggested that the adhesion of zinc oxide (ZnO) nanowires with carbon fibers can significantly improve the interfacial shear strength of fiber-reinforced composites. We have carried out a systematic study of the interaction between ZnO and graphene based on density functional theory, with a focus on the effect of the surface orientation and termination of ZnO. The most thermodynamically stable hexagonal phase of ZnO is modeled by a cluster with (001), (100), and (110) facets, and the (001) surface is constructed to have both Zn-rich and O-rich terminations. The interaction has been explored through varying both the orientation and the binding sites of the interacting surfaces. The interfacial binding strength is calculated by scanning the potential energy surface while bringing the ZnO cluster incrementally closer to graphene. Results from these energy scans will be presented and discussed along with simple physical arguments to rationalize the observed behavior.

Information about the Authors:
This semester the authors had the unique opportunity to partake in a computational physics research class (PHYS-492) offered by Prof. Zygmunt and Prof. He. Over the course of this project, the authors developed modeling and computer programming skills that will come in handy for future graduate studies and explored the less familiar realm of chemical physics. Having previous research experience, each author was able to bring a different piece of knowledge to this project. Allyse Appel is a junior physics major with a concentration in astrophysics and has previously worked with modeling systems; Adam Clark is a junior physics/math double major who has a strong interest in nuclear physics and a background in computer programing; Kelsey Larson is a junior chemistry/physics double major who has a background in physical chemistry and an interest in the dynamics of molecular systems.

Faculty Sponsor: Dr. Haiying He

Student Contact: kelsey.larson@valpo.edu