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**ZnO-Graphene Interfacial Binding Strength: Dependence on Surface Orientation** HAIYING HE, KELSEY LARSON, ADAM CLARK, ALLYSE APPEL, STAN ZYGMUNT, Valparaiso University — There is an increasing interest of hybridized materials with impacts such as improving 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 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. It is found that the calculated interfacial binding strength strongly depends upon the surface orientation and termination of ZnO. Only slight variation in binding energy is observed for different binding sites and Zn/O atoms with different coordination numbers. Comparison of results using a variety of exchange-correlation functionals with different forms of dispersion corrections will be presented.

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