Abstract Submitted
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Analyzing the vdW-DF description of binding mechanisms: Comparison of C60 and benzene adsorption on graphene[1] KRISTIAN BERLAND, PER HYLDGAARD, Chalmers Universtiy of Technology, MATERIALS PHYSICS AND CARBON ENGINEERING TEAM — There has been several efforts to improve the accuracy of the description of sparse matter problems like molecular adsorption on surfaces using non-local correlation functionals. We have explored the vdW-DF [PRL 92, 246401 (2004)] interaction at different length scales, density regimes, density gradients, and for different system. As test calculations, we compare the potential energy curves of benzene and C60 on graphene and related systems like boron nitride because these reveal the role of geometry and band gap on the functional components. Our analysis is facilitated by explicit control of cutoff parameters in our real-space evaluation of the non-local correlation. We find that vdW-DF is very sensitive to the low density regions, but more so for the original version than in the newer one, vdW-DF2 [PRB 82, 081101 (2010)]. Our results also illustrate that a transferable account of many different geometries requires an accurate account of all length scales involved in the problem. These results are discussed in light of the functional form of vdW-DF. We also show how functional choices greatly affects corrugation. Finally, we examine the role of induced dipoles on the adsorption.

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