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Influence of water on the electronic structure of metal supported graphene: Insight from van der Waals density functional theory[1] JI FENG, XIAO LI, ENGE WANG, Peking University, China, SHENG MENG, Institute of Physics, China, JIRI KLIMES, ANGELOS MICHAELIDES, University College London — We investigate the interaction between water and metal supported graphene through van der Waals density functional theory calculations. Our results show a systematic increase in the adsorption energy of water on graphene in the presence of underlying metal substrates. In addition, we find that the electronic nature of the graphene-metal contacts behave differently upon water adsorption: in the case of a weak, physical graphene-metal contact, the charge carrier doping level of graphene is tuned by water, resulting in a Fermi level shift on the order of 100 meV. In the case of a strong chemical graphene-metal contact, the ? and ?* bands of graphene are hardly perturbed by water adsorption. These results illustrate the correlated nature of the interactions between water, graphene, and metal substrates, and show that the electronic structure and the doping level of graphene can be controlled by water deposition.

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