

The hydrophobic to hydrophilic transition of graphene in the presence of H₂O molecules

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In some applications of graphene, for example as electrode materials of supercapacitors and biomaterials supports, it is desirable that graphene is hydrophilic since hydrophilic graphene can improve the interaction between graphene and polar electrolytes or biological molecules. However, pristine graphene is strongly hydrophobic due to the inert nature. Therefore, the development of stable hydrophilic graphene surface is essential for the above applications. This talk presents two different methods to realize this transition based on density functional calculations. It is found that applying external electric field or doping Al atoms into graphene can facilitate the H₂O molecules dissociative adsorption on graphene, thus the presence of OH group on graphene converts graphene to be hydrophilic.

Biography

Zhimin Ao received his Ph.D. in Materials Science from Jilin University, China, in 2008. In 2009, he received the prestigious FWO Postdoctoral Research Fellowship to work as a postdoctoral researcher in the Department of Physics at University of Antwerp, Belgium, from March 2009 to May 2010. His continual high academic performance led him to the highly competitive - the University of New South Wales (UNSW) Vice-Chancellor's Research Fellowship and joined the School of Materials Science and Engineering at UNSW in May 2010. So far, he has published more than 27 papers in peer-reviewed international journals and 3 book chapters. The publications have more than 305 citations. Currently, he is leading a research team on the application of graphene-based materials; he is also a reviewer for several journals, including J. Am. Chem. Soc., Appl. Phys. Lett., J. Phys. Chem. C, Phys. Chem. Chem. Phys., and J. Appl. Phys.

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