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# The hydrophobic to hydrophilic transition of graphene in the presence of $H_2O$ molecules

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## Abstract

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. In this talk, it 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 $H_2O$ molecules dissociative adsorption on graphene, thus the presence of OH group on graphene converts graphene to be hydrophilic.

## Biography

Dr. Zhimin Ao received his PhD degree 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. In June 2013, under the support of highly competitive the University of Technology, Sydney (UTS) Chancellor's Research Fellowship, he joined the Centre of Clean Energy Technology, School of Chemistry and Forensic Science, University of Technology, Sydney, Australia. So far, he has published more than 28 papers in peer-reviewed international journals and 3 book chapters. The publications have more than 385+ citations. Currently, his research focuses on the application of graphene-based materials as hydrogen storage materials and in batteries; 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. etc.