IBS Center for Multidimensional Carbon Materials

Tuesday Colloquium

Prof. Yusong TU

Faculty of College of Physics Science and Technology
Yangzhou University

ystu@yzu.edu.cn

High Correlation between Oxidation Loci on Graphene Oxide

Tuesday, MAY 31
2 PM

Bldg. 101
Seminar room on the 1st floor

Recent experiments have shown the coexistence of both large unoxidized and oxidized regions on graphene oxide (GO), but the underlying mechanism for the formation of the GO atomic structure remains unknown. Now, using density functional calculations, 52 oxidation pathways for local pyrene structures on GO were identified, and a kinetic profile for graphene oxidation with a high correlation between oxidation loci was proposed, which is different from the conventional view, which entails a random distribution of oxidation loci. The high correlation is an essential nature of graphene oxidation processes and can be attributed to three crucial effects: 1) breaking of delocalized p bonds, 2) steric hindrance, and 3) hydrogen-bond formation. This high correlation leads to the coexistence of both large unoxidized and oxidized regions on GO. Interestingly, even in oxidized regions on GO, some small areas of sp2-hybridized domains, similar to “islands”, can persist because of steric effects.

Knowledge of the structure of these regions is of essential importance for understanding and using GO, as unoxidized regions retain characteristic features of graphene, such as hydrophobicity, and its electric and photonic properties. Such knowledge would also facilitate specific graphene functionalization processes with control over the atomic structure for various applications, including energy storage, optoelectronic devices, and biomedicine.

In this presentation, I will discuss our recent advance on understanding the distribution of oxidized groups on the surface of graphene oxides.

You are cordially invited to attend!