Computational Study of Graphene-based Interfaces for the Realization of Next-generation Energy and Electronic Devices

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Abstract

In this talk, I will present our recent research effort in the characterization of graphene-based interfaces for the realization of next-generation energy and electronic devices in collaboration with experimentalists. First, I will discuss the mechanism of high electrocatalytic activity of Se edge-doped graphene nanoplatelets for iodine reduction reaction (IRR) in dye-sensitized solar cells (DSSCs) [1]. The mechanisms of IRR in carbon-based DSSC counter-electrodes are clarified based on density functional theory (DFT) and non-equilibrium Green's function calculations, together with the electrochemical kinetics analysis. Next, I will describe a DFT study of the graphene/WSe2 "barristor" device that shows an exceptional low-temperature characteristic [2]. Combined with the experimental characterization of defect states and device modeling, self-interaction-corrected DFT calculations reveal a novel charge transport mechanism originating from trap-assisted tunneling rather than the typical thermionic emission process. If time permits, I will close the talk by mentioning the DFT study of high-performance Li battery realized with TiO2 anatase nanoparticles adsorbed on graphene, in which we provide the atomistic picture of the "domino cascade" Li ion insertion process [3].

References

[1] M. J. Ju, et al. Sci. Adv. **2** (2016) e1501459.
[2] J. Shim et al., Adv. Mater. **28** (2016) 5293.
[3] G. H. Lee et al., Adv. Funct. Mater. (available online, DOI: 10. 1002/adfm. 201601355).

Figures