Boron and Nitrogen Doped Graphene Used as Counter Electrode for Iodine Reduction in Dye-Sensitized Solar Cells

Kuan-Yu Lin (林冠宇)[1], Jyh-Chiang Jiang (江志強)[1]
1. Department of Chemistry Engineering, National Taiwan University of Science and Technology, Taipei, Taiwan

A counter electrode (CE) which acts as an efficient catalyst, has a pivotal role in dye-sensitized solar cells (DSSCs). As graphene and its derivatives exhibit high conductivity [1], optoelectronic properties, hardness, and stability in corrosive electrolyte, we considered them for use as a CE. Using density functional theory (DFT) calculations on both gas phase and at solid surfaces, our results demonstrated that a parallel adsorption of I_2 on the doubly boron-nitrogen doped graphene (BNG) surface is more favored than on the pure and boron-doped graphene (BDG) surfaces. The doubly doped BNG surface provides several active sites, large electron transfer, and more efficient electrocatalytic activity, even though the corresponding adsorption energy is not the largest one. The negatively charged BNG surface is able not only to strongly capture the I_2 molecule but also to lower the energy barrier for iodide reduction. The energy barriers for the I_2 dissociation on the negatively charged BNG and BDG surfaces amount to 0.4 and 0.8 eV, respectively. The present findings suggest that the negatively charged BNG surface emerges as a promising candidate for replacement of the Pt-based counter electrode catalysts in the DSSC devices. It is desirable that appropriate experimental study of Pt-free CE catalysts using carbon-based nanomaterials with low cost and high efficiency advantages could be implemented.

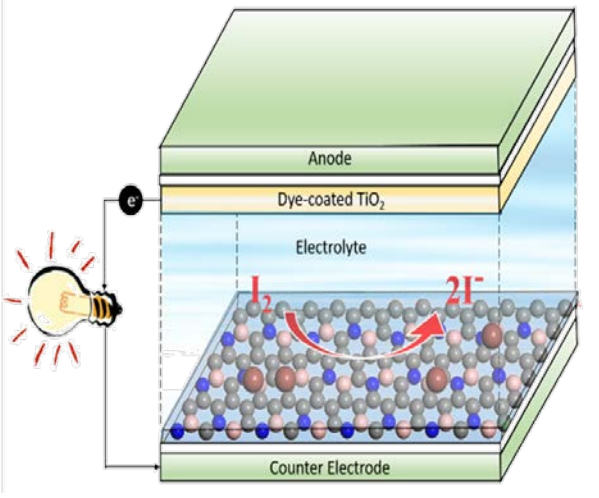

Figure 1. Schematic of DSSCs using Boron-Nitrogen-Codoped Graphene (BNG) as CE

References

[1] Cai X., Lv Z. B., Wu H. W., Hou S. C. and Zou D. C., J. Mater. Chem. **2012**, 22, 9639.

Email: D10606002@mail.ntust.edu.tw