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Materials Research Society-Taiwan

Invited speaker's information form of IUMRS-ICA 2017

Presentation on Symposium F2:
Materials Design, Discovery, and Optimization Based on Computation

Presentation title: Lithiation Mechanism and Lithium Storage Capacity of Reduced Graphene Oxide Nanoribbons – A First-Principles Study

Speaker's name and affiliation: Chin-Lung Kuo, National Taiwan University

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Brief biography of Speaker:

Prof. Chin-Lung Kuo received his B.S. and M.S. degree in Chemical Engineering from National Taiwan University in 1994 and 1996, respectively, and then the Ph.D. degree from Cornell University in 2005. From 2005 to 2007, he conducted his postdoctoral research at the University of Texas at Austin. Afterwards, he joined the Department of Materials Science and Engineering at National Taiwan University in August 2007. His current research interests mainly focus on employing molecular modeling and simulation techniques to develop atomistic understandings of the structures and the structure-property relationships for various materials systems. Based on these fundamental understandings developed, we can further investigate the underlying mechanisms of complex materials phenomena and many fundamental aspects that remain unknown and controversial to date, which are useful in guiding the rational design and synthesis of novel materials for the future technology node.

Abstract:

We employed first-principles calculations to investigate the lithiation mechanisms of functionalized graphene nanoribbons (GNRs) and to examine the effect of various functional groups on the electrochemical performance of graphene-based nanomaterials. In this work, we have extensively explored the Li storage behaviors of various types of functional groups located on the basal plane and those terminating the edge sites within different levels of lithiation and functionalization on GNRs. For functional groups terminating the edge sites, only ketone and its related derivatives (pyrone/quinone) can effectively enhance Li adsorption on GNRs, and the most favorable sites for Li adsorption turn out to be these edged-oxidized groups rather than the hollow sites on the basal plane. In addition, as the ketone-terminated GNRs were fully lithiated, the Li/O atomic ratio was found to be ~1.0 and that for the ketone-ether pair (pyrone) was ~0.5, indicating that these edge-oxidized groups can effectively enhance the Li capacity of GNRs as compared with that of graphite (Li1/6C). As regards the in-plane functional groups, the epoxy and hydroxyl groups were shown to have multiple Li uptakes on the basal plane and appeared to serve as the nucleation centers for Li clustering, thereby resulting in the great enhancement of the Li capacity of GNRs. Our calculations showed that the achievable Li/O atomic ratio was 4 for the epoxy group (Li4O pyramid cluster) and 3 for the hydroxyl group (Li3(OH) cluster), respectively, which suggest that these in-plane functional groups can be more effective in enhancing the Li storage capacity than those terminating the edge sites of graphene-based nanomaterials.

Please fill the above form and send it to Prof. Shih-kang Lin (linsk@mail.ncku.edu.tw), Prof. Nien-Ti Tsou (tsounienti@gmail.com), and Prof. Chih Chen (chih@mail.nctu.edu.tw).