Contribution ID: **315** Type: **Poster**

First Principles Study of Structural Stability and Electronic Band Structure of Al2C Monolayer and Nanotube

Thursday 25 May 2017 17:45 (15 minutes)

Excitonic solar cells (XSC) based on heterojunction nanostructure composed of low-dimensional materials have gained a great deal of interest due to its large interface area and hence the high possibility in generating excitons. In general, the power conversion efficiency (PCE) of this XSC depends strongly on the interface band alignment between donor and acceptor materials. Therefore, low-dimensional materials with adjustable band alignment are highly desirable for achieving high PCE applications. Among many candidates, Al_2C monolayer(s) with band gap of 1.05 eV has been proposed as a suitable material for photovoltaic applications. The similar expectation is also paid for Al_2C nanotube as it possesses even higher surface area ratio. However, structural stability and band gap of the nanotube have not been reported yet, even though there has been assumption that it may be possible to tune the band gap by varying nanotube radius. Therefore, in this work, we use density functional theory based on generalized gradient approximation (GGA) and hybrid functional (HSE06) to investigate structural stability and band gap of both Al_2C monolayer and nanotube. From the results, both GGA and HSE06 band gaps of Al_2C monolayer agree well with previously reported data, which confirms the validity of our calculations. Then, for the Al_2C nanotube, we found that its band gap is somewhat sensitive to the size and the helicity of nanotube. Specifically, the band gap for zigzag (n,0) nanotube vanishes (i.e. the metallic state) when nanotube diameter (d) is reduced to about 8.0 Å. On the other hand, the band gap for zigzag (0,n) nanotube increased to about 1.2 eV under the decrease of nanotube diameter to 7.5 Å. Furthermore, at small diameter limit (d < 20 Å), the strain energy as a function of nanotube radius indicates that Al_2C nanotube is even more stable than the widely studied SiC_2 nanotubes. With radius dependence, the wide range and adjustable band gap of Al_2C nanotube provide its capability to be tuned in obtaining suitable/desired band alignment for enhancing PCE of XSC.

Authors: Mr PRAMCHU, Sittichain (Department of Physics and Materials Science, Faculty of Science, Chiang Mai University); Dr JAROENJITTICHAI, Atchara (Department of Physics and Materials Science, Faculty of Science, Chiang Mai University); Dr LAOSIRITAWORN, Yongyut (Department of Physics and Materials Science, Faculty of Science, Chiang Mai University)

Presenter: Mr PRAMCHU, Sittichain (Department of Physics and Materials Science, Faculty of Science, Chiang Mai University)

Session Classification: Poster Presentation II

Track Classification: Statistical and Theoretical Physics