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## First Principles Study of Structural Stability and Electronic Band Structure of Al<sub>2</sub>C Monolayer and Nanotube

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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<sub>2</sub>C 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<sub>2</sub>C 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<sub>2</sub>C monolayer and nanotube. From the results, both GGA and HSE06 band gaps of Al<sub>2</sub>C monolayer agree well with previously reported data, which confirms the validity of our calculations. Then, for the Al<sub>2</sub>C 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<sub>2</sub>C nanotube is even more stable than the widely studied SiC<sub>2</sub> nanotubes. With radius dependence, the wide range and adjustable band gap of Al<sub>2</sub>C nanotube provide its capability to be tuned in obtaining suitable/desired band alignment for enhancing PCE of XSC.

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