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Graphene/Transition metal oxides thin films using first principle approaches

Thursday, 28 June 2018 15:00 (2 hours)

Since the effectively increase in the efficiency of dye sensitized solar cells (DSSCs) by O'Regan and Gratzel in 1991, the research in the string of DSSCs has grown rapidly. The preparation of the mesoporous oxide (typically, titanium dioxide) film is a key factor in the optimization of DSSCs because of its enormous influence on the anchoring of dye molecules, and the transfer and separation of charge carriers. However charge recombination is a main negative factor that limits DSSCs performance. It is predicted that improving the conduction from the location of the photo-generated carriers to the collecting electrode would considerably enhance the DSSC efficiency. One way to slow recombination is by use of composite semiconductor photoanode with different bandgaps.

Recently, carbonaceous nanomaterials such as carbon nanotubes and two-dimensional graphene sheet have attracted the attention of the scientific community in probe to improve energy conversion and storage technologies. The graphene sheet is more preferred due to its large specific area, flexible structure, high transparency and also excellent mobility of charge carriers and is expected to be able to slow the charge recombination. Graphene/Transition metal oxides nanocomposite study has become much of a wide interest recently with metal oxides like titanium dioxide, zinc oxide, Chalcopyrite, etc in search to improve the DSSCs performance. The final composite embodies both the transport properties of the former and the semiconducting properties of the latter species. This talk gives preliminary results of electronic and optical properties of the final composite studied using the Density Functional Theory in application to DSSCs.

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