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Electrochemical property of carbon nanotubes, graphene oxide and reduced graphene oxide: First-principles and experiment

Zijun Shi and **Yanfang Gao**
Inner Mongolia University of Technology, China

By the look of development, first-principles electronic structure calculations are a powerful tool to elucidate microscopic details of structures and properties in electrochemical field. In this work, we reported the electrochemical performance of carbon-based materials by first-principles calculation, which are based on DFT were performed using CASTEP and DOML3 program (Materials Studio7.0). We make the best of the theoretical calculation demonstrated that band gap of carbon nanotubes (CNT), graphene oxide (GO) and reduced graphene oxide (rGO) are 0.500eV ,3.328eV and 0.144eV, respectively. Showed that rGO electrochemical performance is better than CNT and GO, furthermore , we also investigated by means of electrochemical experiments. Specifically, the specific capacitance of CNT, GO and rGO are 45.27 F g^{-1}, 0.608 F g^{-1} and 238.8 F g^{-1}, respectively, at a current density of 1 A g^{-1}. Its outcome can directly describe the remarkable electrochemically active of rGO as well. In addition, by theoretical calculation showed that the existence of a great deal of epoxy groups affects the electronic structure, further expand the range of electrochemical application for rGO. For these purpose, rGO with unique structure and outstanding properties will become the intriguing carbon materials in supercapacitors, owing to avoid π-π stacking and van der waals interactions, the application of electrochemical may be controlled by adjusting content of oxygen, contain tiny amounts of band gap which can vastly enhance the potential in various applications.

18247183702@163.com