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Evaluating the performance of graphene with structural defect and functionalized by $-C_6H_4$ as an electrode active material for supercapacitors

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Abstract

In this study, quantum capacitance of graphene-based electrodes is evaluated using Density Functional Theory (DFT) calculations. The obtained results showed that quantum capacitance of graphene-based supercapacitors could be significantly improved by existence of structural defects on the graphene sheets at sufficiently high concentrations because of creating impure states resulted from carbon p_z orbitals involved in defect. In another section of calculations, quantum capacitance of functionalized graphene with $-C_6H_4$, is evaluated. The obtained results of calculations showed that functionalized graphene with this functional group have a very good capacitance in comparison with pristine graphene, especially at smaller voltages of less than -1.0 V or greater than 1.0 V. Hybrid configurations between structural defects and functional group of $-C_6H_4$ was also studied. In general, the results indicated that the combined configuration shows higher capacity than pristine graphene.

Keywords: supercapacitor, functionalized graphene, DFT calculations, quantum capacitance

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