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Electrochemical performance of 1D carbon nanotubes and 2D graphene-based materials: First-principles and experiment

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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 based on DFT were performed using CASTEP and DOML3 program (Materials Studio 7.0). 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 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 band gap can vastly enhance the potential in various applications.

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Entangled fractal clusters forming the lattice animals in irreversible DLCA binary systems

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Irreversible diffusion limited cluster aggregation (DLCA) of binary sticky spheres was simulated by modifying the Brownian Cluster Dynamics (BCD). We randomly distribute N spheres in a 3D box of size L, the volume fraction is given by $\Phi_{tot}=\pi/6$ (N_{tot}/L^3). We identify N_A and N_B number of spheres as species A and B in our system both having identical size which undergoes Brownian motion. Irreversible bond formation happens only between intra-species particles, while inter-species particle interact only through hard core repulsions. We observe bigels for certain fraction of A particles. In our study the fraction of B particles is kept greater than A particles, so that B species always percolate (cluster size equal to L) while species A do not percolate below a critical fraction which varies with volume fractions. Thus, by tuning the volume fraction and fraction of A and B particles we were able to regulate the size of the cage and thereby were able to design clusters of a specific size. The aggregation kinetics is well explained by Smoluchowski rate equation. We will also show that the accessible volume of the system increases when compared to the monomeric case, which means that species A is aggregating inside the cage created by B. Contrary to monomeric DLCA we observe that for moderate Φtot both the species undergo a transition from lattice animal to the percolation region. This can be observed by the fact that there is a change in fractal dimension from 2 to 2.5 which we have also verified by cluster size distribution. We will also show that A clusters are stuck inside the B percolating cluster and always have a fractal dimension of 2, thus having 2 characteristic length scale for binary system. We will also show that diffusion of one species of particles is hindered by the presence of the other species forming cages.

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