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Investigation of Energy Storage Capabilities of Graphene and h-BN Double Layer Electrostatic Supercapacitor

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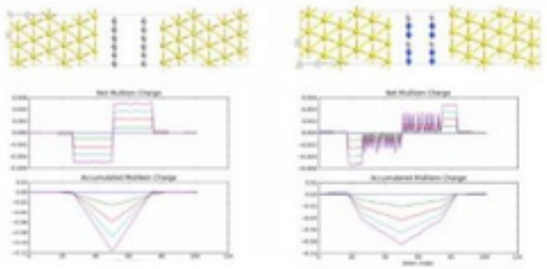
In this study, graphene and hexagonal boron nitride (h-BN) sheets were investigated theoretically as 2-dimesional planar electrodes in nano size capacitors. Quantum capacitance and energy storage capacities of perfect (pristine) model systems formed in different geometries and shapes will be reported. Quantum mechanical calculations were performed using the Density Functional Theory (DFT) based Non-equilibrium Green's Function (NEGF) method. By providing convergence, the quantum transport quantities as well as the charge distributions and the capacitance of the system can be found. Calculation of the capacitance properties of the electrode-device-electrode systems was carried out using ATK (Atomistix ToolKit) package program. The non-polarized GGA / PBE + NEGF approach was used in the calculations. The wave functions are expressed by the basic sets of DZP (Double-Zeta-Polarized), which are local numerical atomic trajectories. Structural optimization of the working systems was done by the Fast Inertial Relaxation Engine (FIRE) method. The preliminary results obtained by Mulliken analysis are $2.18\text{x}10^{-20}$ F ($0.18\text{x}10^{-20}$ F) for quantum capacitance, 3.37 μF/cm^2 (2.26 μF/cm^2) for spesific capacitance and 29.64 F/g (45.61 F/g) for gravimetric capacitance of graphene (h-BN) model capacitor system.



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Synthesis of Poly(Azomethine)s Derived From Dialdehyde and Phenazopyridine Hydrochloride: Characterization, Thermal and Spectroscopic Studies

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An alternate method to synthesize conjugated polymer is the use of azomethine (–N=C–) connections. Conjugated poly(azomethines), polyimines, or poly(Schiff bases) are another interesting class of conjugated polymers containing nitrogen atoms in a polymer backbone.[1] Among the rich chemistry of various semiconductors, the conjugated compounds with CH=N Schiff base linker, seem to be attractive for opto-electronics. The main representatives of this family are azomethines, also named Schiff bases or imines. [2,3] Poly(azomethine)s possess the ability to form liquid crystals and complexes with metals, are characterized in terms of high thermal stability and exhibit therapeutic activity, therefore they are widely used in different fields such as analytical chemistry, organic synthesis, medicine, biology, as well as in organic electronics as electrochromic material and photovoltaic (OPV) cell components. [4]

In this study, two poly(azomethine)s were prepared via polycondensation chemistry in which two formerly synthesized dialdehydes were reacted with phenazopyridine hydrochloride to give a Schiff base polymer in a simple one-step process of polycondensation.

The chemical structure of the synthesized compounds was characterized by the FT-IR, UV-Vis, ^{1}H-NMR and ^{13}C-NMR techniques. Further characterization was employed using thermogravimetric analysis-differential thermal analysis (TG-DTA), fluorescence (PL), electrochemical-cyclic voltammetry (CV) and differential scanning calorimetry (DSC) measurements. The number of average molecular weights of polymers was calculated using GPC instrument. Scanning Electron Microscopy (SEM) images were illustrated to explore the morphologic property.

1. Adams R., Bullock J. E. Wilson W. C. (1923). Journal of American Chemistry, 45, 521-527.
2. Koole M., Frisenda R., Petrus M. L., Perrin M. L., van der Zant H. S. J., Dingeman T. J. (2016). Organic Electronics, 34, 38-41.
3. Barik S., Bletzacker T., Skene W. G. (2012). Macromolecules, 45 (3), 1165-1173.
4. Bolduc A., Mallet C., Skene W. G., (2013). Science China Chemistry 56 (1), 3-23.