597c Modeling Porous Carbons by Reverse Monte Carlo and Simultaneous Energy Minimization

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We present a simulation protocol to build atomistic models for disordered carbons. The original Reverse Monte Carlo (RMC) technique[1] consists of randomly changing the positions of an array of carbon atoms in a box to generate a three-dimensional configuration that is consistent with X-ray or neutron diffraction results. The uniqueness of the original RMC method has been questioned in the literature[2]. To overcome this uniqueness problem, normally constraints are used in the RMC procedure. However, it has been reported in the literature that the models obtained from RMC may contain some high energy structures, such as 3 and 4 member rings, which are unphysical. We overcome this problem by introducing an energy penalty term in the RMC procedure. The energy penalty term reduces the probability of having high energy structures in the resultant models and correctly describes the local environment of the carbon atoms. We use an empirical bond-order potential developed by Brenner[3] to model the interactions between carbon atoms and between carbon and hydrogen atoms. We perform the simultaneous RMC and energy minimization by using the minimization technique known as simulated annealing[4].

We used our simulation protocol to generate models for a group of porous carbons that fits the experimental structure factor. We characterized the resulting models by calculating the geometrical pore size distribution, ring statistics, surface area and by performing Grand Canonical Monte Carlo simulations in order to obtain the nitrogen adsorption isotherm at 77 K.

References:

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