Grand Canonical Monte Carlo Simulations of Hydrogen in Carbon Nanostructures

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In this work we studied hydrogen uptake in carbon matrices by means of Monte Carlo simulations in the Grand Canonical ensemble (GCMC), with generalized Lennard-Jones intermolecular potentials. We used as a substrate nanostructured carbon films (na-C) obtained by simulating the deposition of cluster beams. Adsorption isotherms reveal that the different nanostructure does not significantly affect \(\text{H}_2\) storage process. By combining \(\text{H}_2\) physisorption and atomic \(\text{H}\) chemisorption the hydrogen uptake we obtained is in very good agreement with what what experimentally determined in na-C by a recent spectroscopic study.