Abstract Submitted
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Adsorption of hydrogen in boron-substituted nanoporous carbons[1] L. FIRLEJ, U Montpellier 2, B. KUCHTA, U Provence, S. ROSZAK, Wroclaw U Technology, P. PFEIFER, C. WEXLER, U Missouri — Nanoporous carbons are promising for hydrogen storage. However, the heat of physisorption is low (4.5-8 kJ/mol), which limits the total amount of hydrogen adsorbed at room temperature to ˜2 wt.% at 100 bar. To enhance sorption the surface must be modified by substitution or doping/intercalation of some atoms in the carbon skeleton by other elements. Here we present coupled *ab initio* calculations and Monte Carlo simulations showing that partial substitution of carbon atoms in nanoporous matrix with boron increases significantly the adsorption energy (up to 10-13.5 kJ/mol) and storage capacity (˜5 wt.% at 298 K, 100 bar), even for relatively low substitution ratios (5-10%). Although substitution causes both energetic and structural heterogeneity of the adsorbent, at room temperature the delivery of the stored gas during adsorption-desorption cycle is almost complete (˜97 %). We analyze whether the location of substituted atoms (within the graphene plane or between two adjacent planes) and randomness of its distribution modify either the adsorption mechanism or/and storage parameters. In particular the heterogeneity of energy landscape is discussed in a context of optimization of system delivery.

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