Abstract Submitted
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Structural and energetic factors in designing a perfect nanoporous sorbent for hydrogen storage[1] BOGDAN KUCHTA, Université de Provence, LUCYNA FIRLEJ, Université Montpellier 2, RAINA CEPEL, PETER PFEIFER, CARLOS WEXLER, University of Missouri — Carbons are one of potentially promising groups of materials for hydrogen storage by adsorption. However, the heat of hydrogen physisorption in such materials is low, in the range of about 4-8 kJ/mol which limits the total amount of hydrogen adsorbed at P = 100 bar to ∼2 wt% at room temperature and about ∼10 wt% at 77 K. To get better storage capacity, the adsorbing surfaces must be modified, either by substitution of some atoms in the all-carbon skeleton by other elements, or by doping/intercalation with other species. Here we analyze the variation of interaction energy between a molecule of hydrogen and graphene-based sorbents prepared as hypothetical modifications of the graphene layer. In particular, we show that partial substitution of carbons (for example, by boron) modifies both the symmetry of the energy landscape and strength of hydrogen physisorption. The effect of substituent extends over several sites of graphene lattice making the surface more heterogeneous.

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