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Multi-scale modeling of hydrogen energy storage by adsorption on new graphene related materials

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Graphene planes functionalized by hydrogen or fluor atoms can constitute the characteristic adsorptive surfaces of new porous materials. Structure and symmetry of the atom arrangements in graphane and fluoro-graphene have been estimated from experiments and ab-initio computations. These data allow to determine the molecular interactions between gas molecules and the functionalized graphene materials by ab-initio calculations or to describe them by approximate effective atom-atom potentials. In this work on the basis of such interactions and potentials, we calculate by Monte-Carlo simulations the adsorption properties of hydrogen on graphane and fluoro-graphene. Comparison of simulation results shows that the two sets of molecular interactions data are in good agreement. The adsorption is obtained up to high pressure and temperature 293 and 77 K. The hydrogen total adsorption on fluoro-graphene is 40 % higher than that on graphane. The total weight percent of hydrogen storage at 77K on fluoro-graphene seems around 9 %.

Keywords: