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Study on the Adsorption of Small Gas Molecules on graphene by the Density Functional Theory Calculations YIMING MI, Graduate Department, Shanghai University of Engineering Science, 333 Longteng Rd., Shanghai 201620, PR CHINA, XINXIN ZHAO, School of Fundamental Studies, Shanghai University of Engineering Science, 333 Longteng Rd., Shanghai 201620, PR CHINA, SHUICHI IWATA, Graduate School of Frontier Sciences, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8654, JAPAN — The absorption of different small gas molecules on graphene is investigated based on the pseudopotential method within the density functional theory formalism. The preferred adsorption site (among the top, bridge, and hollow positions) and orientations of these molecules on the graphene surface are analyzed and the related adsorption energies are calculated. The charge transfer between the absorpted molecules and the graphene is discussed as well.

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