新学術領域「コンピューティクスによる物質デザイン：複合相関と非平衡ダイナミクス」
公募研究「シリコン中原子空孔の量子状態シミュレーション」

Title: First-Principles Calculations of Hydrogen Impurities in Carbon Nanomaterials

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By using first-principles electronic structure calculations, we study hydrogen monomers and dimers in the graphene, armchair edge (5,5) carbon nanotube (CNT) and zigzag edge (10,0) CNT. We find that the monomers in the the above three carbon nanomaterials have the magnetic moment of $1\mu_B$. In the case of the CNTs, the hydrogen atoms are located on the outer side of the CNTs. In the most stable structures of the dimers in the above three carbon materials, two hydrogen atoms are bonded to host carbon atoms which are nearest neighbors. In the case of the graphene, two atoms are located on the opposite sides whereas in the case of the armchair edge (5,5) CNT and zigzag edge (10,0) CNT, both two hydrogen atoms are located on the outer side. The electronic structures of the most stable geometries are found to be nonmagnetic. However, when the two hydrogen atoms are bonded to second nearest carbon atoms, the magnetic moment is found to be $2\mu_B$.