

I-N Electronic Properties of Nanostructured Materials

I-N-1 Carbon Foam: Spanning the Phase Space between Graphite and Diamond

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We study an unusual class of carbon structures, based on rigidly interconnected segments of graphite. The resulting foamlike systems cover the structural phase space extending from hexagonal diamond to graphite. Related to the most stable phases of carbon, these hybrid systems show an unusually high structural stability at low mass densities. Our density-functional calculations indicate that carbon foam is metallic, stable, and structurally rigid.

I-N-2 Electronic Structure of Ba₄C₆₀ and Cs₄C₆₀

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We study the electronic structure of body-centered-orthorhombic Ba₄C₆₀ superconductor and Cs₄C₆₀. In both fullerenes, it is found that the band structure is metallic and that the low symmetry of the lattice gives rise to the lifting of the threefold degeneracy of t_{1u} and t_{1g} bands even at the Γ point. We study also the electronic structure of Cs₄C₆₀ under pressure and find it to be a promising candidate of a superconducting Cs fulleride.

I-N-3 Geometric and Electronic Structure of New Carbon-Network Materials: Nanotube Array on Graphite Sheet

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We design a new class of carbon network materials with a periodically modified graphite sheet. The modified part corresponds to (6,6) carbon nanotube geometry. Their tube parts form triangular lattice on graphite sheet. On these systems each tube has six heptagons at the bottom, giving rise to a seamless sp^2 -C network with a negative curvature. We consider these nanotube arrays on graphite sheet with three kinds of tube-end geometries and various sizes for both graphite and tube parts. We report their electronic structure obtained by using a realistic tight-binding model, and for selected systems the density-functional theory. Interestingly, results show that most of them are semiconductors although both (6,6) tube and graphite are metallic. The difference in their tube-end geometries

and the sizes of graphite and tube parts affect their electronic structures. Some have nearly flat band states around the Fermi level, showing a possibility of ferromagnetic behavior if hole or electron is doped. Some are direct-gap semiconductors whose interband transition is optically allowed. Their typical gap energies are about 1 eV. Therefore they should emit infrared light.

I-N-4 First Principles Study of H₂ and CH₄ Physisorption on Carbon Nanotubes

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We study the energetics of physisorption of H₂ and CH₄ molecules on the single-walled carbon nanotube (SWNT) using the local density approximation in the framework of the density-functional theory. The radius of the studied nanotube is 4.69 Å, around the average size of the mass-produced SWNTs. Both inside and outside-wall physisorption processes with various molecular directions and adsorption sites are studied, and compared to those on a flat graphite sheet. It is found that H₂ and CH₄ molecules are generally stably adsorbed on the inside wall as well as on the outside wall. The energy gain upon physisorption of the H₂ on the inside wall of a carbon nanotube is about 0.10 eV, while that of CH₄ is about 0.17 eV. For the CH₄ adsorption, the energy gain depends considerably on a molecular direction. H₂ molecule is also stably adsorbed on the interstitial channel (IC) of the nanotube bundle, and the energy gain is about 0.19 eV. The Adsorption-site dependence is strong in the case of the H₂ adsorption on the outside wall of a nanotube and on the IC of nanotube bundles.