

Abstract Submitted
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Novel electronic properties of hydrogenated graphene: A first-principles calculation HONG-YAN LU, RUI WANG, SHIH-YANG LIN, C. S. TING, Texas Center for Superconductivity and Department of Physics, University of Houston, Houston, Texas 77204, USA — We studied the electronic properties of some new kinds of hydrogenated graphenes by first-principles calculations. The designed systems, depending on the position and concentration of the hydrogen atoms, may show interesting band structures that are different from that of the pure graphene. For example, we can obtain semiconductor of a gap about 3eV with flat valance and conduction bands, or semimetal with anisotropic Dirac cones in which the position of Dirac points are shifted from K points, or semimetal with flat band crossing the Dirac cone at the Dirac point. The consequences of these features will be presented. We are able to get good metal with considerable density of states at Fermi level. The phonon dispersions and spectra as well as the electron-phonon couplings of such metallic systems are currently being investigated by the first-principles calculation, their superconductivity transition temperatures T_c should thus be predictable by assuming the electron-phonon coupling as the pairing interaction. We expect that the phonon frequencies are quite large, and the T_c could be high for some of the metallic systems.

Hong-Ya
Texas Center for Superconductivity and Department of Physics, University of Houston, Houston, Texas 77204,

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