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Novel electronic properties of hydrogenated grapheme: The first principles calculations

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Fully- and semi-hydrogenated graphene, named graphane (C_6H_6)[1,2] and graphone (C_6H_3)[3,4], were previously found to be nonmagnetic semiconductor with a direct gap of 3.5 eV and antiferromagnetic semiconductor with an indirect gap of 2.46 eV, respectively. Here, by means of first-principles calculations, we predict other kinds of partially hydrogenated graphene systems[5]: C_6H_1 and C_6H_5, which are ferromagnetic (FM) semimetal and FM narrow-gaped semiconductor with an indirect gap of 0.7 eV, respectively. When properly doped, the Fermi surface of the two systems consists of an electron pocket or six hole patches in the first Brillouin zone with completely spin-polarized charge carries. If superconductivity exists in these systems, the stable pairing-symmetries are shown to be p+ip for electron doped case, and anisotropic p+ip for hole doped case. The predicted systems may provide fascinating platforms for studying the novel properties of ferromagnetism and triplet-pairing superconductivity. In addition, the electronic structures of hydrogenated graphene C_6H_2 and C_6H_4 have also been studied. We find that C_6H_2 is a Dirac semimetal with 2 highly anisotropic cones located well inside the first Brillouin zone, and C_6H_4 is a semiconductor with a gap of ~3.35 eV. A detailed discussion of their properties will be presented.

Biography

C S Ting is a Professor of Physics at the University of Houston. His major research area has been on theoretical condensed matter physics including transport theories in various solid state systems, superconductivity in copper oxide materials and iron pnictides, magnetism, metal-insulator transition, electronic property of graphene, solids with the spin-orbit couplings and strongly correlated electron systems. He is the Principal Investigator in Theory at the Texas Center for Superconductivity at the University of Houston, and a Fellow of APS in the Division Condensed Matter Physics.

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