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Effects of Carbon Doping in MgB_2 and Boron Doping in Diamond

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We will present doping effects on two famous superconductors, MgB_2 and B-doped diamond, using first principles electronic structure studies of two types-the ordered supercell method and the coherent potential approximation (CPA) method which incorporates disordered effects. First, in MgB_2 which has a real possibility for a high field conductor as well as a high critical temperature, a detailed analysis of the changes in electronic structure and the effective σ-band doping. The occupied local density of states of C is almost identical to that of B in the upper 2 eV of the valence band, but in the range -8 to -2 eV, C has a considerably larger density of states. Our calculations indicate that the cylindrical σ Fermi surfaces pinch off at the zone center above the 10% C-doping. Second, in B-doped diamond with maximum T_c~12K for 4.7 % boron concentration, our calculated coupling strength λ~0.5 leads to T_c ~5-10K, and indicates that the cause of the superconductivity is the same as the origin of hardness, very strong carbon-carbon bonding. The CPA bands, broadened somewhat reflecting the disorder-induced lifetime, are consistent with angle-resolved photoemission spectroscopy (ARPES) band maps. The B character is 1.7 times larger than for C per atom near the top of the valence bands.

Keywords : MgB_2, B-doped diamond, First principle calculations, CPA

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Reference:

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