ELECTRON-PHONON COUPLING IN ICOSAHEDRAL BORON-RICH SOLIDS

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In this work, I will focus on the understanding gained from the investigation of the strength of the electron-phonon coupling in icosahedral boron-rich solids with theoretical methods based on the density functional theory and on the density functional perturbation theory [1]. In particular, icosahedral boron carbides are hard ceramics, and the idea of combining this hardness and the superconductivity has emerged. I will show results on the electron-phonon coupling in $B_{13}C_2$ [1] and our recent results in α-boron under high pressure [2].

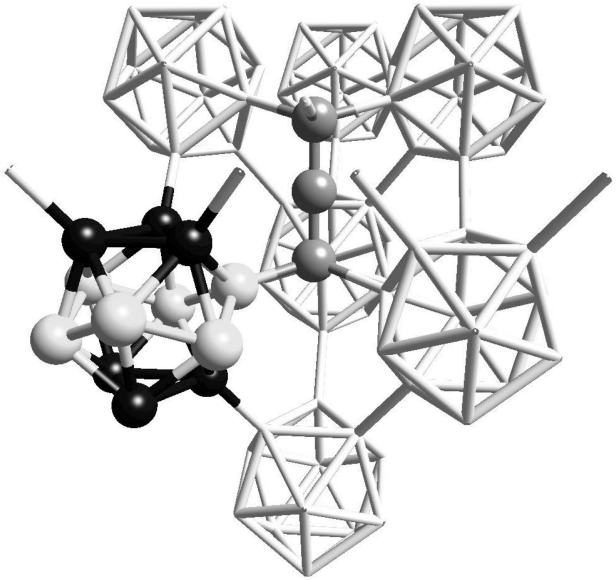

Figure 1. Atomic structure of an icosahedral solid : boron carbide B_4C . Distorted icosahedra $B_{11}C$ are bonded to each other either directly, or through a triatomic C-B-C chain. Black balls : atoms in the polar site. White balls : atoms in the equatorial site. Grey balls : atoms of the triatomic chain. According to our calculations, hole-doping of B_4C leads to $B_{13}C_2$*, a superconducting metallic phase.[2]*

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