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The effects of hydrogenation and high pressure on α-tetragonal boron: a first principles study NAOKI UEMURA, KOUN SHIRAI, ISIR, Osaka University — It is well known that boron rich crystals are superhard materials. α-tetragonal (α-tet) boron is one of the metastable phase in elemental boron crystals under high temperature and high pressure. This phase has a possibility of including some hydrogen atoms due to the experimental process, but it has not yet been shown crystal structures and electronic properties of hydrogenated α-tet boron. Using first-principles calculations, we theoretically predicted stable structures and investigated the influences from hydrogenation of α-tet boron and high pressures. According to our calculations, non-bonding states of pure α-tet boron, which were mostly occupied by P_z like orbitals coming from interstitial boron atoms in α-tet boron, were completely vanished by doping some hydrogen atoms and the higher the pressure was, the lager energy gaps between the valence band maximum and the conduction band minimum on α-tet boron were. These results provide that the deformation potential depended on the pressure is positive, which is basically negative on semiconductors except for diamonds and is an index of the hardness under pressure on semiconductors.

Naoki Uemura
ISIR, Osaka University

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