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Structural and electronic properties of the half-Heusler phases PtFeBi, PtMnBi, PdFeBi and PdMnBi XIAOFANG WANG, XIAOSHUANG CHEN, Shanghai Institute of Technical Physics, Chinese Academy of Sciences, CHINGYAO FONG, Department of Physics, University of California, Davis, WEN-CHAO HUANG, WEI LU, Shanghai Institute of Technical Physics, Chinese Academy of Sciences — First-principles calculations based on density functional theory have been performed to study the structural and electronic properties of the PtFeBi, PtMnBi, PdFeBi and PdMnBi half-Heusler alloys. The results reveal that all the alloys show metallic properties at the ground state configuration. We further investigated the dependence of electronic band structures by applying hydrostatic pressure. It is found that the PtMnBi and PdMnBi are half-metallic with the same magnetic moment of 4.0 μB per formula-unit when their lattice constants are reduced (from -3.0% to -11.2% and -6.1% to -7.9%, respectively). For PtMnBi, its band gap of the minority spin channel increases with compression due to the noticeable strong p-d hybridization, which is the reason for the formation of bonding and antibonding states. It is obvious that the high spin polarization of PtMnBi is over a large range of its lattice constant and with a wide band gaps in the PtMnBi. However, the PdFeBi and PtFeBi are quasi-half-metallic with magnetic moment to be 3.0 μB at -6.9% and -8.3% uniform strain, respectively. They are sensitive to the changes of lattice constants.

Xiaoshuang Chen
Shanghai Institute of Technical Physics, Chinese Academy of Sciences

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