Enhanced Spin Polarization at $n$-MnSb(0001)/InP(111) Interface

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Abstract—We studied the electronic and structural properties of the interfaces between the niccolite ($n$-) polymorph of ferromagnetic MnSb and the binary semiconductor InP along the MnSb(0001)/InP(111) direction. Plane-wave pseudopotential ab-initio electronic structure calculations were used. The Mn-to-P interface becomes 63.0% spin-polarized, much higher than the bulk polarization. The other three possible interfaces for contacts retain their ferromagnetism at the interface. Adhesion energy of the Mn-to-P interface is 63meV/ Å, larger than the other terminations, and it has the shortest interlayer bond distance of 2.43 Å. The high interface spin polarization of the favorable Mn-to-P interface is advantageous for spin transport.