FIG. 1. (Color online) Top: the lattice constants a of YBrI as a function of U. Bottom: the energy band structures of YBrI without SOC and U=0 eV.
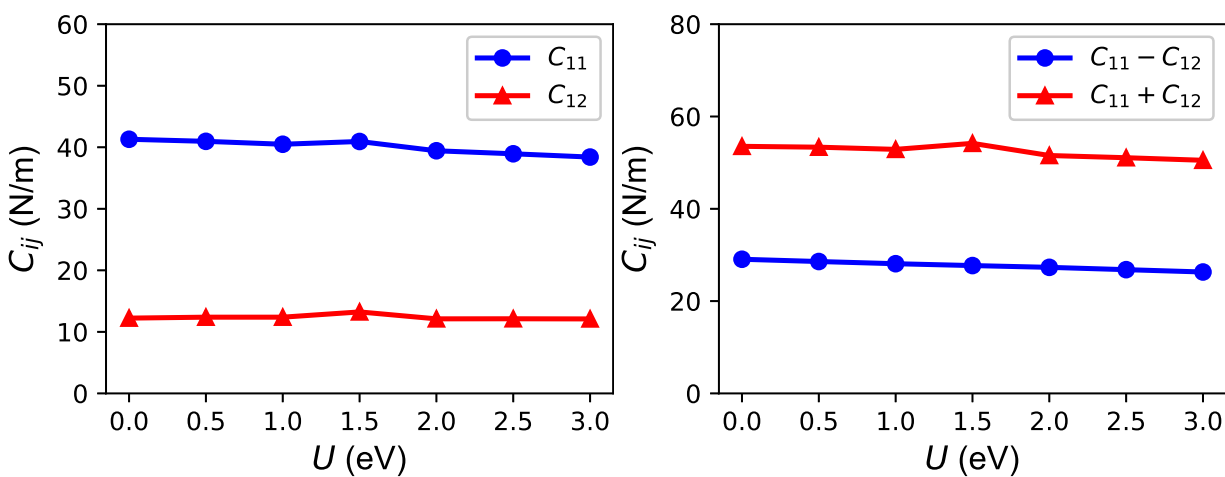

FIG. 2. (Color online) For monolayer YBrI, the elastic constants C_{ij} as a function of U.
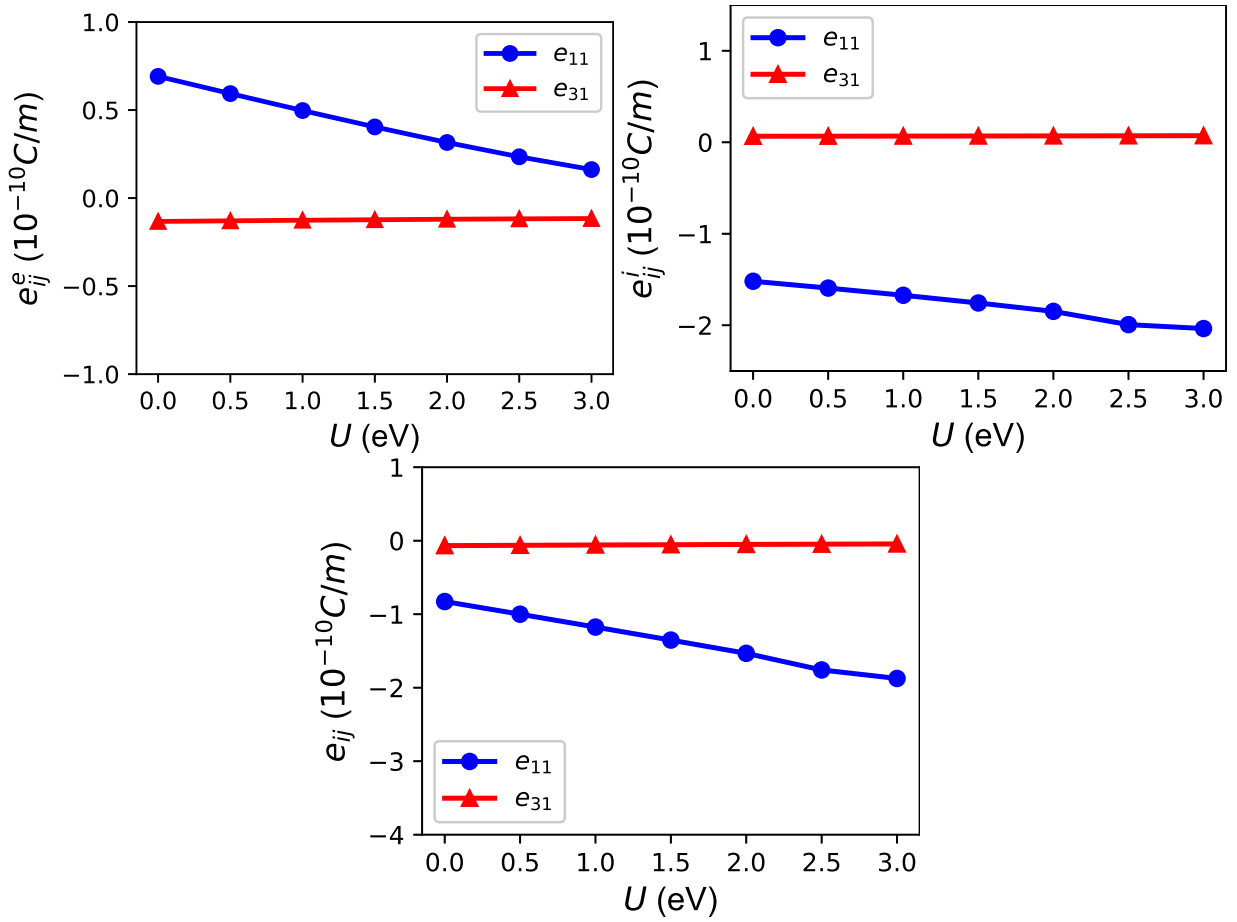
FIG. 3. (Color online) For monolayer YBrI, the piezoelectric stress coefficient (e_{ij}) along with the ionic contribution and electronic contribution as a function of U.
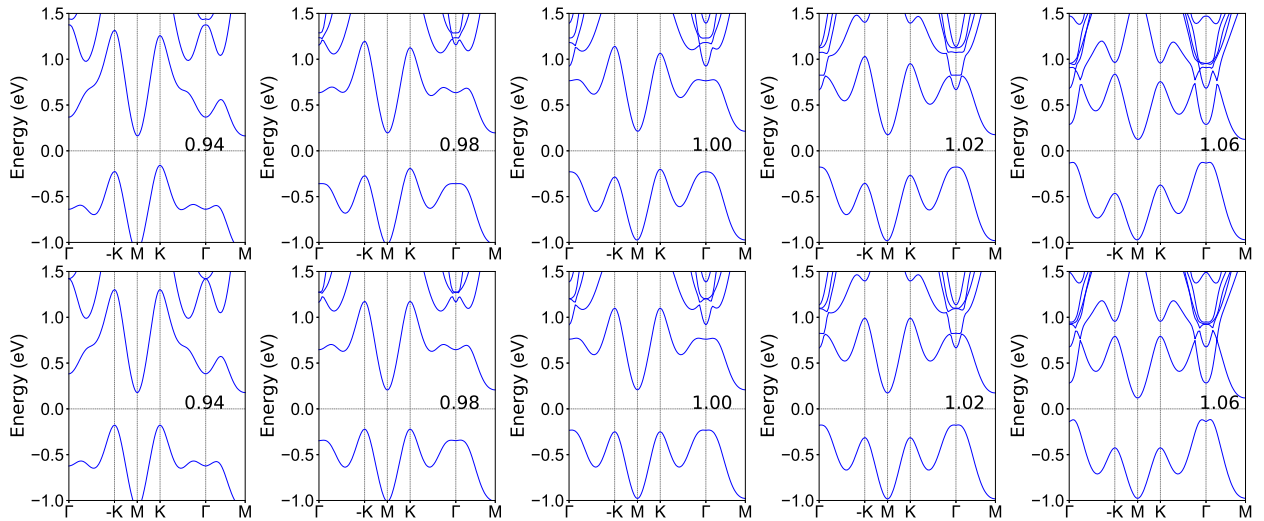

FIG. 4. (Color online) The energy band structures of YBrI monolayer with out-of-plane (Top) and in-plane (Bottom) magnetic anisotropy by using GGA+SOC at some representative a/a_0 values.
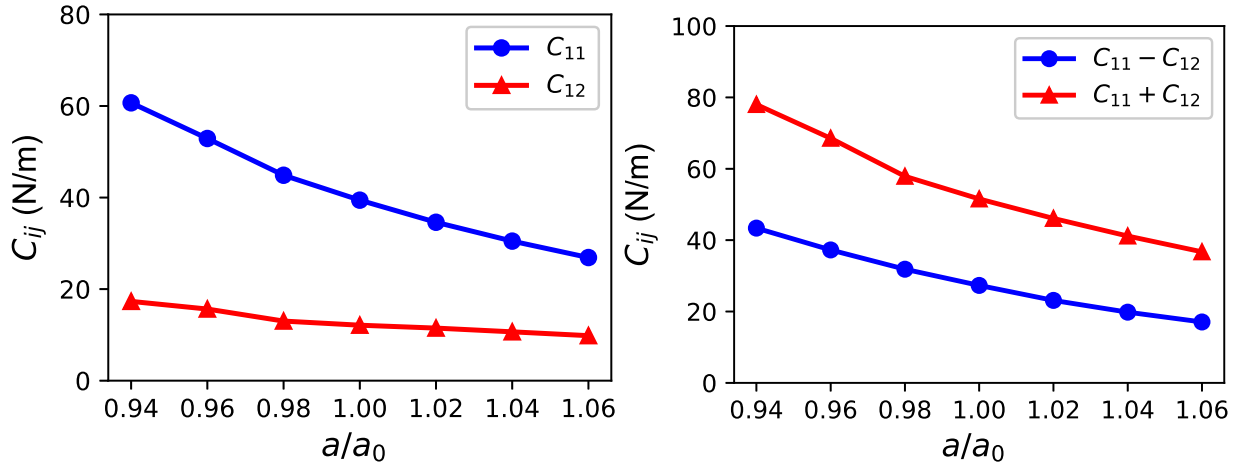
FIG. 5. (Color online) For monolayer YBrI, the elastic constants C_{ij} as a function of a/a_0.
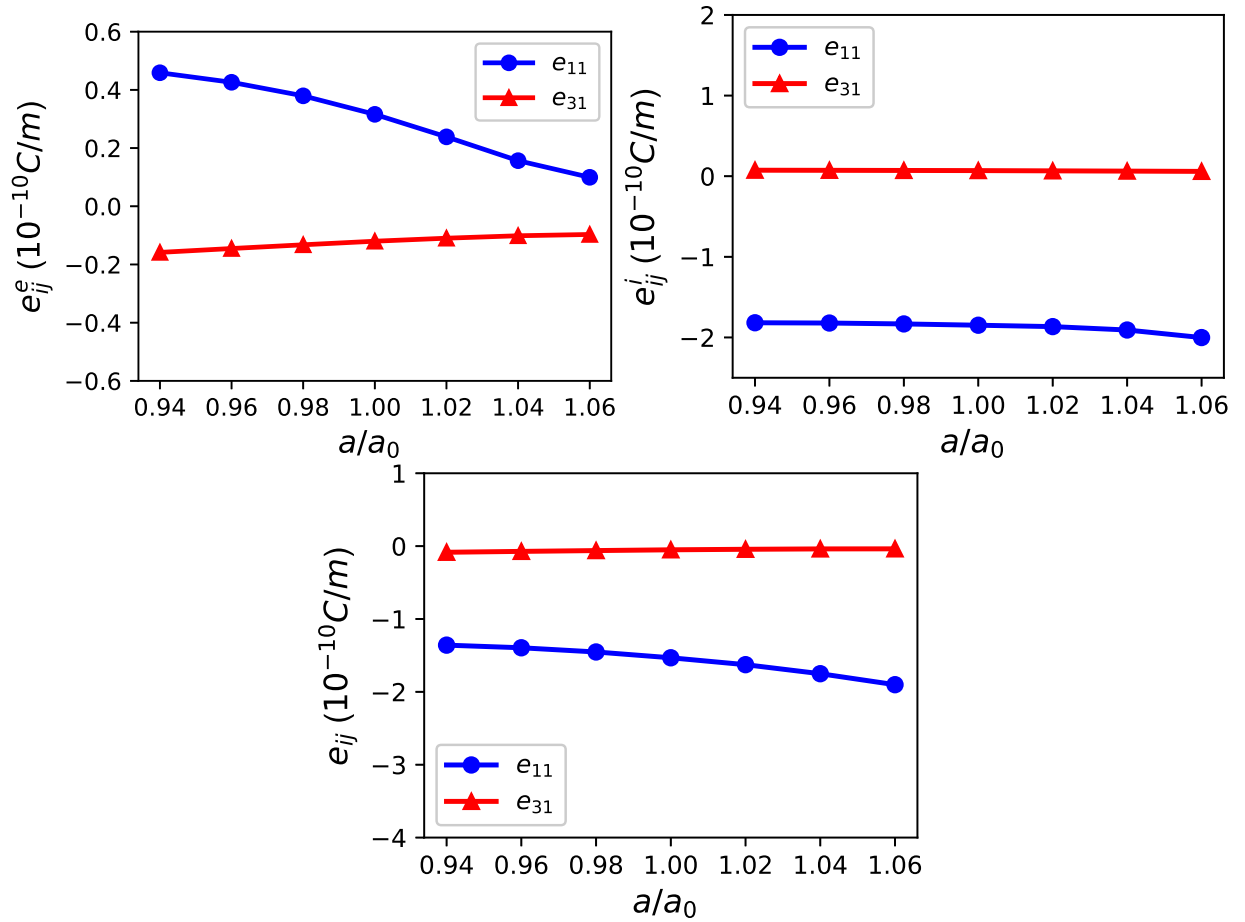

FIG. 6. (Color online) For monolayer YBrI, the piezoelectric stress coefficient (e_{ij}) along with the ionic contribution and electronic contribution as a function of a/a_0.
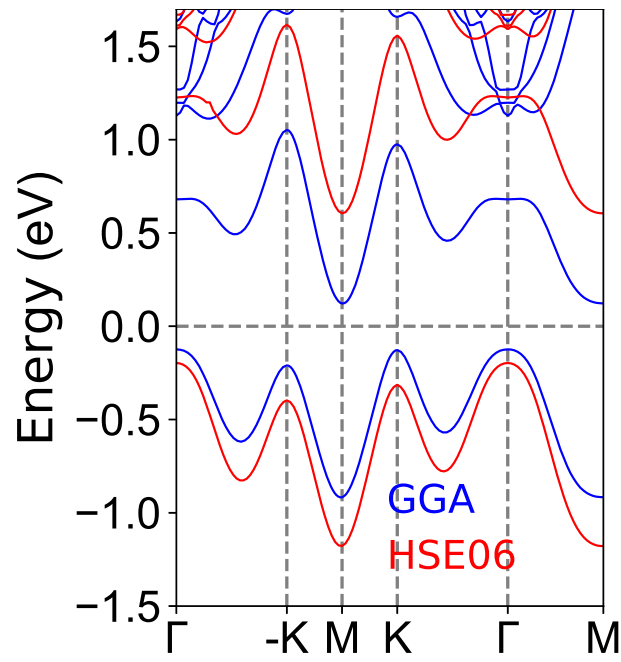
FIG. 7. (Color online) By using GGA+SOC and HSE06+SOC, the energy band structures of YBrI with out-of-plane case.