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Electronic properties of CH3NH3PbBr3 (001) surface XIN HUANG, TULA PAUDEL, University of Nebraska-Lincoln, SHUAI DONG, Southeast University,China, EVGENY TSYMBAL, University of Nebraska-Lincoln — The energetics and electronic properties of cubic CH3NH3PbBr3 (001) surfaces are studied using a first-principles method. We find that the uncompensated intrinsic dipole moment of a CH3NH3 molecule induces a band bending, being larger for the PbBr2-terminated surface than for the CH3NH3Br-terminated surface. When the intrinsic dipole are fully compensated, the surface electronic structure shows new states near band edges for both MABr and PBBr2 terminations. We find that for the PbBr2-terminated surface, less dispersive surface states appear just above the bulk valence bands at the center of Brillouin zone (Γ? point), while for the CH3NH3Br-terminated surface, more dispersive surface states appear below the conduction bands at the M point. These states effectively reduce the band gap and improve optical absorption properties. The PbBr2-terminated surface states are of the Pb-p character, and hence are strongly affected by spin-orbit coupling, whereas the CH3NH3Br-terminated surface states are of the Pb-s character and hence are not affected by the spin-orbit coupling effect. Our study suggests a way to tune the spin-orbit coupling by selecting an appropriate surface.

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