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Electronic Structure and Stability of the $\text{CH}_3\text{NH}_3\text{PbBr}_3$ (001)

Surface TULA R. PAUDEL, Department of Physics and Astronomy & Nebraska Center for Materials and Nanoscience, University of Nebraska, Lincoln, NE 68588, XIN HUANG, Department of Physics, Southeast University, Nanjing 211189, China, PETER DOWBEN, Department of Physics and Astronomy & Nebraska Center for Materials and Nanoscience, University of Nebraska, Lincoln, NE 68588, SHUAI DONG, Department of Physics, Southeast University, Nanjing 211189, China, EVGENY TSYMBAL, Department of Physics and Astronomy & Nebraska Center for Materials and Nanoscience, University of Nebraska, Lincoln, NE 68588 — The energetics and the electronic structure of methylammonium lead bromine ($\text{CH}_3\text{NH}_3\text{PbBr}_3$) perovskite (001) surfaces are studied based on density functional theory. By examining the surface grand potential, we predict that the $\text{CH}_3\text{NH}_3\text{Br}$ -terminated (001) surface is energetically more favorable than the PbBr_2 -terminated (001) surface, under thermodynamic equilibrium conditions of bulk $\text{CH}_3\text{NH}_3\text{PbBr}_3$. The electronic structure of each of these two different surface terminations retains some of the characteristics of the bulk, while new surface states are found near band edges which may affect the photovoltaic performance in the solar cells based on $\text{CH}_3\text{NH}_3\text{PbBr}_3$. The calculated electron affinity of $\text{CH}_3\text{NH}_3\text{PbBr}_3$ reveals a sizable difference for the two surface terminations, indicating a possibility of tuning the band offset between the halide perovskite and adjacent electrode with proper interface engineering.

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