Supplementary Information

■ Calculation methodology

The first-principles calculations were performed using density functional theory (DFT) methodologies implemented in the Vienna ab-initio simulation package (VASP).[1, 2] The generalized gradient approximation (GGA) was used for the exchange correlation functional in a form suggested by Perdew, Burke, and Ernzerhof (PBE),[3, 4] and a cutoff energy of 400 eV was used. Electron-ion interactions were treated with the projector augmented wave (PAW) method.[5, 6] The parameter settings in the calculations were as follows: the force criteria on the atoms was less than 0.02 eV/Å, and the energy variation was less than 1×10^{-5} eV per atom. The surface slabs were separated by a vacuum region of 15 Å, which is large enough to prevent the artificial interaction between the distinct slabs. The valence configurations were $4d^{10}5s^{1}$ for Ag and $4s^{2}4p^{5}$ for Br. In order to better describe the band structures, the GGA+U formalism was incorporated in the DFT calculations; the U values were chosen as $U_{d, Ag}$ = 1.6 eV and $U_{p, Br}$ = 1.3 eV.[7] Spin-polarized DFT calculations were applied in this study to obtain the lattice parameters, and electronic density of states (DOS) was calculated using tetrahedron method with Blöchl corrections for AgBr (100) and AgBr (111). The AgBr (100) surfaces were modeled by 6-atom-layer slabs which represent 2 × 2 lateral cells with all atoms were relaxed, and the AgBr (111) surfaces were modeled by 11.5-atom-layer slabs (O-terminated) which represent 2 × 2 lateral cells with all atoms being relaxed.

■ Results and discussion

The densities of states (DOS) of two different surfaces were calculated by DFT methodologies (see Fig. S1). After the alignment with respect to electronic levels of bulk atoms, the conduction-band minimum (CBM) position of AgBr (111) was found to be higher than that of AgBr (100) by 0.099 eV, very consistent with the result of Mott-Schottky analysis. This result implies that the photogenerated electrons would transfer from the {111} facets to the {100} facets when the facet heterojuction of {100} and {111} facets is formed.

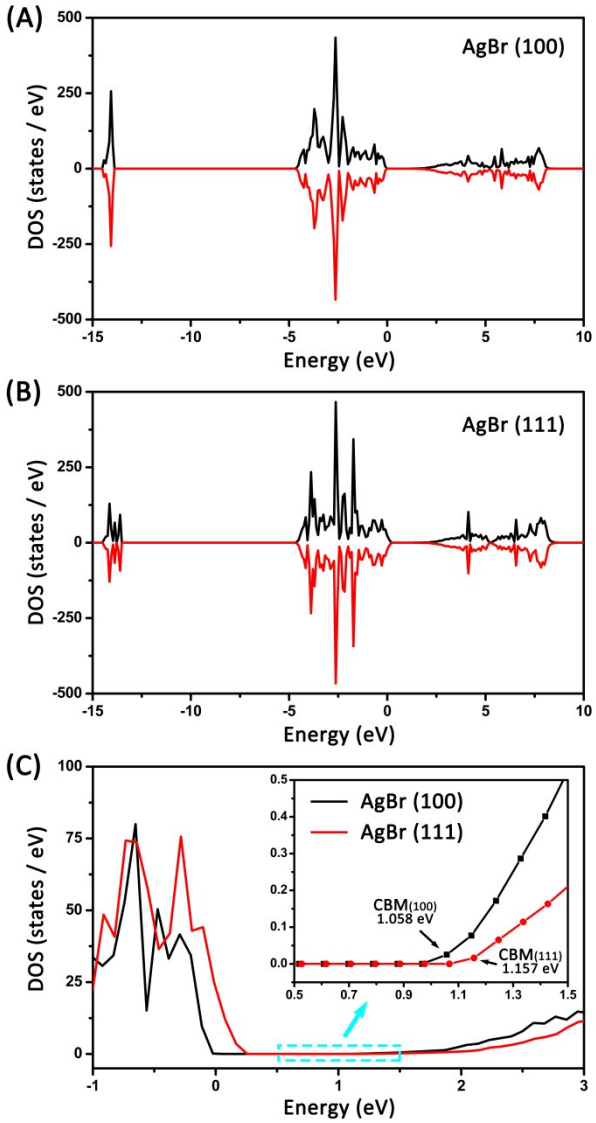

Fig. S1. Calculated densities of states for (A) AgBr (100) and (111) surfaces. (C) Enlarged DOS region for AgBr (100) (black) and AgBr (111) (red).

References

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