Electronic supplementary information

A theoretical exploration of structural feature, mechanical, and optoelectronic properties of Au–based halide perovskites $A_2Au^IAu^{III}X_6$ (A = Rb, Cs; X = Cl, Br, I)

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Computational details

The power conversion efficiency η of an absorber layer can be defined as $\eta = P_m/P_{in}$, where P_m is the maximum output power density and P_{in} is the total incident solar power density. The P_m can be derived by numerically maximizing J (the current density) × V (voltage). The J for a solar cell illuminated under the photon flux I_{sun} is given by the equation $J = J_{SC} - J_0(1 - e^{eV/kT})$ (k is the Boltzmann's constant and T is the temperature). The short-circuit current density J_{sc} is defined as $J_{SC} = e\int_0^{\infty} A(E)I_{sun}(E)dE$, where e, $A(E)$, and $I_{sun}(E)$ are the elementary charge, the photon absorptivity, and the standard AM1.5G solar spectrum at 300 K, respectively. The reverse saturation current J_0 ($J_0 = J_0^{nr} + J_0^{r} = J_0^{r}/f_r$) corresponds to the total electron-hole recombination current density at equilibrium in the dark. The fraction of radiative recombination current f_r is computed by the expression $f_r = \exp(\frac{E_g - E_g^{da}}{kT})$, where E_g and E_g^{da} are the fundamental and direct allowed band gaps, respectively. The J_0^r is calculated from the rate black-body photon absorption from the surrounding thermal bath through the front surface $J_0^r = e\pi\int_0^\infty A(E)I_{bb}(E,T)dE$, where $I_{bb}(E, T)$ is the black-body spectrum at room temperature. The $A(E)$ can be obtained from the relation $A(E) = 1 - e^{-2a(E)L}$, where L and $\alpha(E)$ are the film thickness and the absorption spectrum of the material, respectively. In addition, the open-circuit voltage V_{OC} is determined by the relationship $V_{OC} = \frac{kT}{e}\ln(1 + \frac{J_{SC}}{J_0})$. Finally, the maximum η of a material can be evaluated once two parameters $\alpha(E)$ and f_r are obtained.