Mobility Driven Thermoelectric and Optical Properties of Two-Dimensional Halide-based Hybrid Perovskites: Impact of Organic Cation Rotation

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Figure S1. Projected density of states (PDOS) with the projection of I-5(pₓ, pᵧ and pₜ) and Pb-6(pₓ, pᵧ and pₜ) orbitals for each MA cation rotation in Pb-I network. Fermi level located at 0 eV.
Figure S2. Charge density iso-surfaces (for HOMO and LUMO level) (without SOC) with MA cation rotation.
Figure S3. Part of the valence band structure (along the $\Gamma$-X-Y high symmetry direction of BZ for A1-A4 and R1-R5 structures) calculated with spin-orbit coupling (SOC) effects for visualization of Rashba splitting with the rotation of MA cation.
Figure S4. SOC-Projected density of states (PDOS) (a) Pb-6p and (b) I-5p orbitals including spin orbit coupling effects for A1-A4 structures (symmetric rotation of MA cation) and R1-R5 (Random rotation of MA cation). Fermi level located at 0 eV.
The electrical conductivity and Seebeck coefficients have been calculated using BoltzTrap code through following expressions:

\[ S_{\alpha\beta}(\varepsilon, T, \mu_c) = \int_{-\infty}^{\infty} g(\varepsilon)(\varepsilon - \mu_c) \left[ -\frac{\partial f(T, \varepsilon, \mu_c)}{\partial \varepsilon} \right] d\varepsilon \]

\[ \sigma_{\alpha\beta} = \frac{1}{\Omega} \int \sigma_{\alpha\beta}(\varepsilon) \left[ -\frac{\partial f_{\mu_c}(T; \varepsilon)}{\partial \varepsilon} \right] d\varepsilon \]

where \( \sigma_{\alpha\beta}(\varepsilon_{l,k}) = e^2 \tau_{l,k} v_{\alpha}(i, k) v_{\beta}(i, k) \), while \( g(\varepsilon) \) determines the transport function. Here, \( \varepsilon_{l,k} \) represents the band energy for \( l^{th} \) band at \( k \) wavevector, \( \alpha \) and \( \beta \) are the components of the conductivity tensor, while \( \mu_c, T \) and \( \Omega \) depicts the chemical potential, temperature and volume of cell.

References