Supporting Information

Atomically thin two-dimensional hybrid perovskites using hydrophobic superalkali cations with tunable electron transition type

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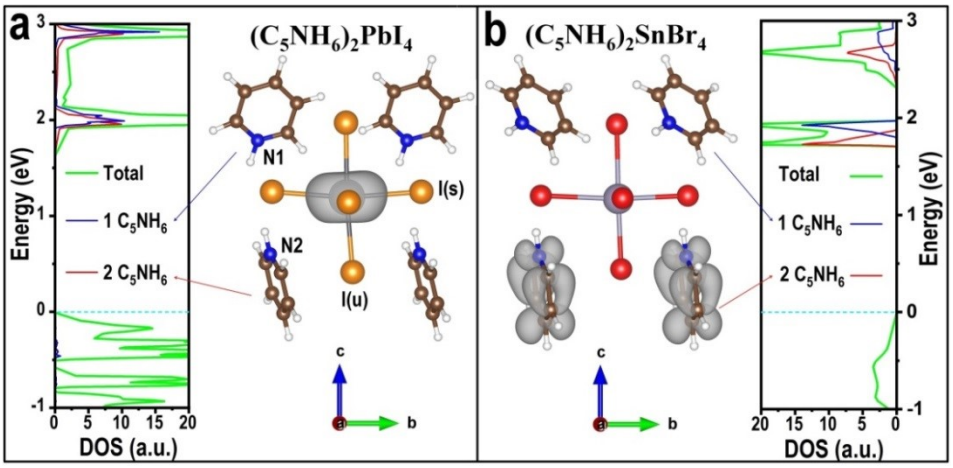

Fig. S1. The total/partial DOSs and the CBM (grey) charge density of the 2D (a) $(C_5NH_6)_2PbI_4$ and (b) $(C_5NH_6)_2SnBr_4$ with an unit cell, respectively. Atomic colors: H (white), C (coffee), N (blue), Br (red), I (orange), Sn (silver), and Pb (grey).

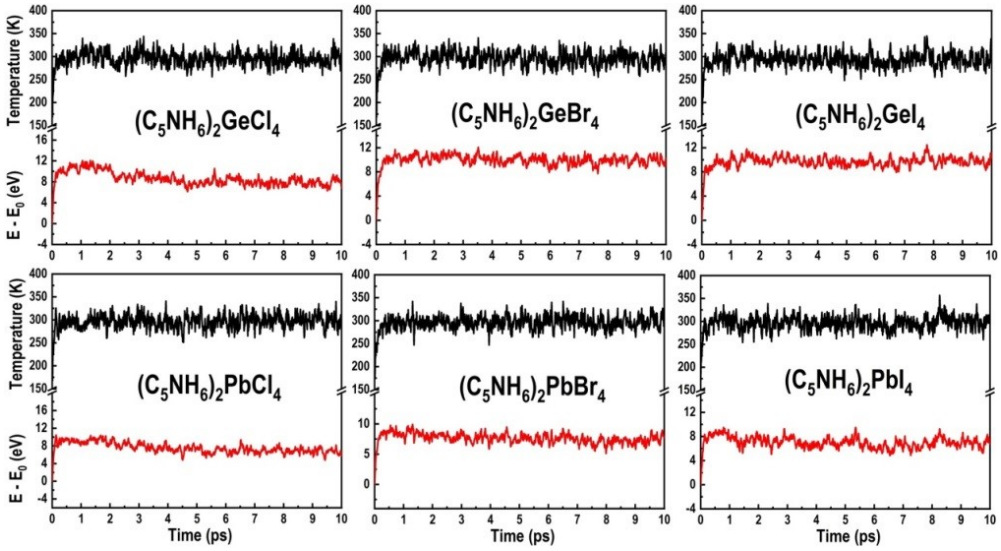

Fig. S2. The AIMD simulated energy and temperature curves of the 2D perovskites with a 3×3×1 supercell under 300 K and 10^5 Pa.

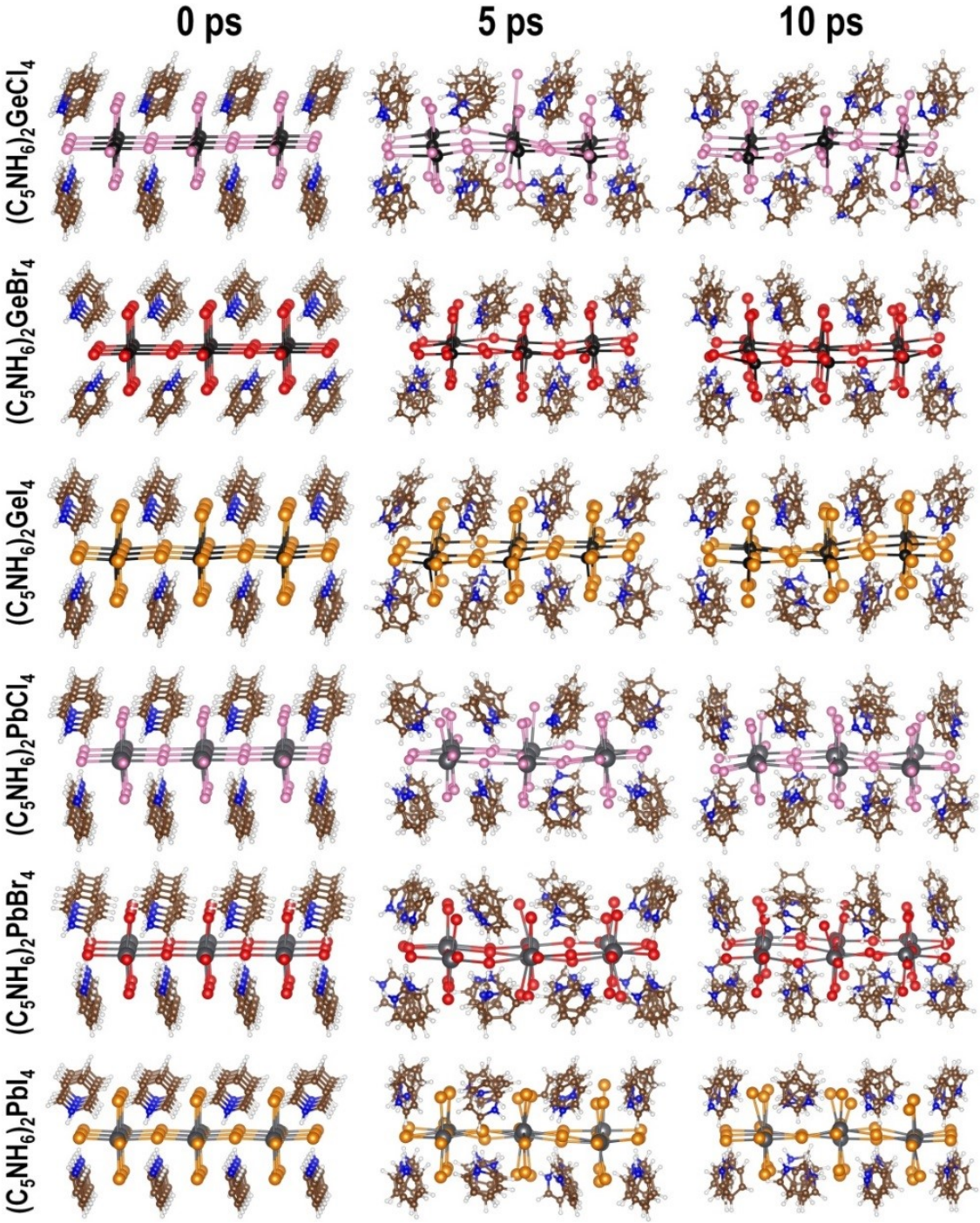

Fig. S3. The AIMD simulated structures of the 2D perovskites with a 3×3×1 supercell under 300 K and 10^5 Pa, respectively. Atomic colors: H (white), C (coffee), N (blue), Cl (pink), Br (red), I (orange), Ge (black), and Pb (grey).

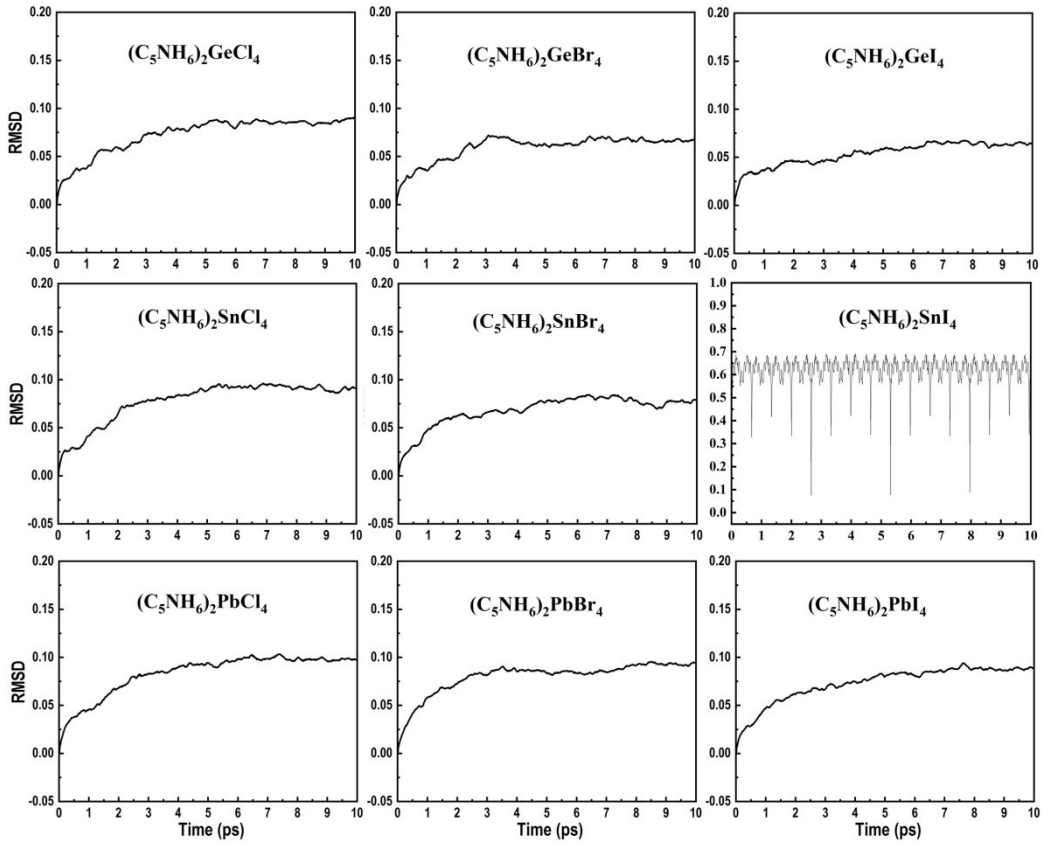

Fig. S4. The root mean square deviation (RMSD) of the 2D perovskites.

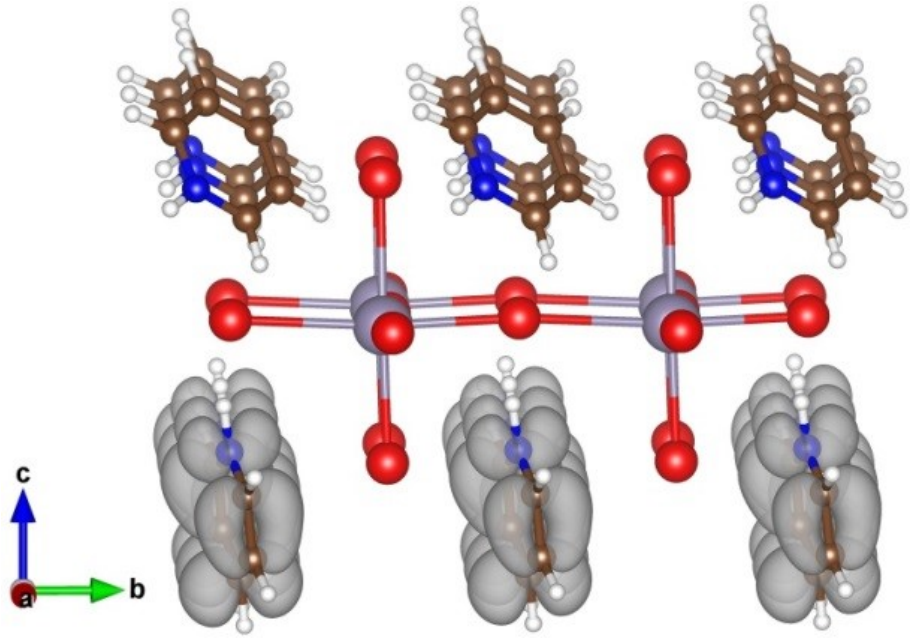

Fig. S5. The CBM (grey) charge density of the 2D $(C_5NH_6)_2SnBr_4$ with a 2×2×1 supercell. Atomic colors: H (white), C (coffee), N (blue), Br (red), and Sn (silver) (grey).

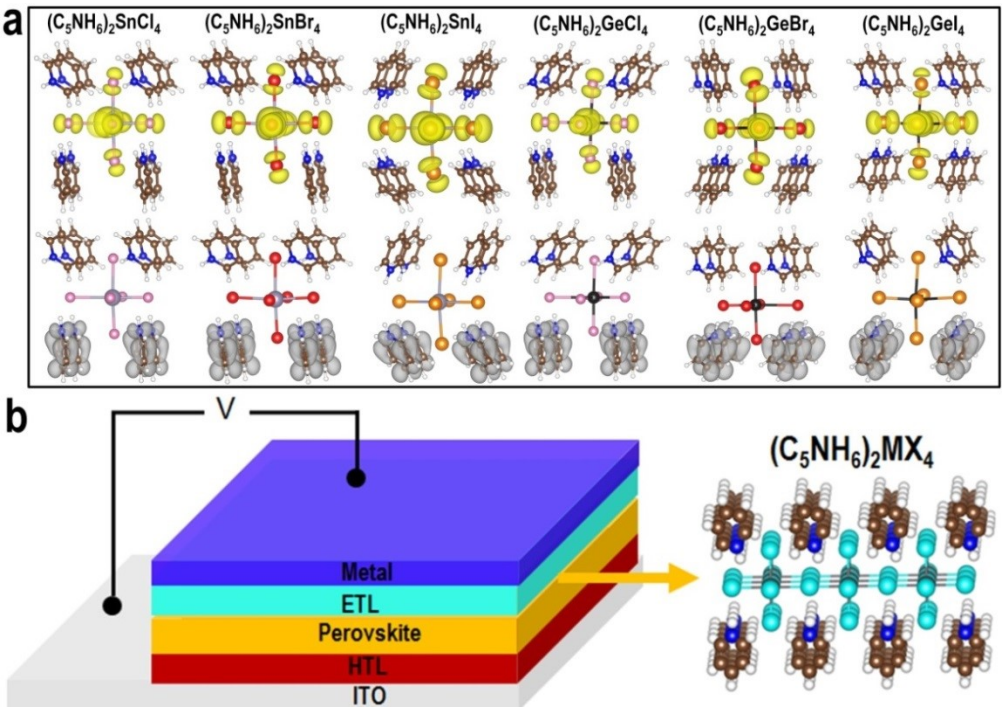

Fig. S6. (a) The charge density of VBM (yellow) and CBM (grey) states for the 2D $(C_5NH_6)_2Sn/GeX_4$ perovskites (isovalue = 0.002 e/Å^3). (b) The model of the light-emitting diode. ITO, HTL and ETL represent indium tin oxide, hole and electron transport layers, respectively. Atomic colors: H (white), C (coffee), N (blue), Br (red), I (orange), and Ge (black), and Sn (silver).