Structural and optoelectronic properties of quasi 1D hybrid 3-halogenopyridinium lead bromides

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Supplementary information

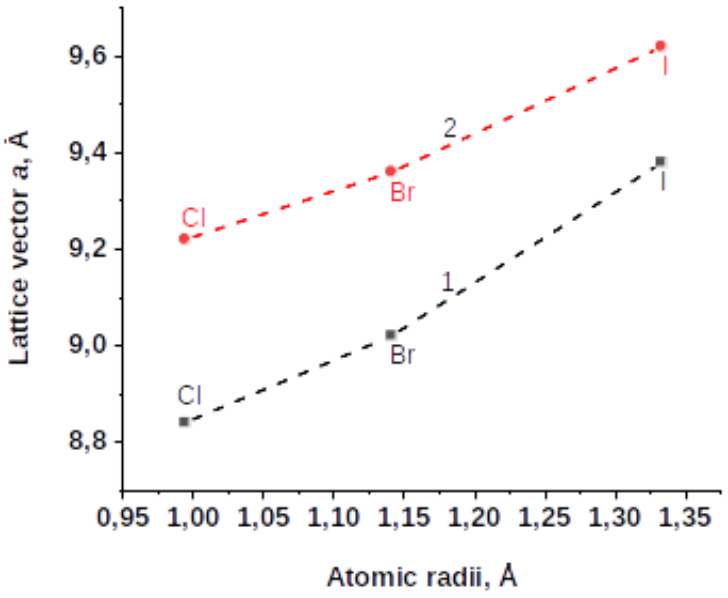

Figure S1. The length of crystallographic ***a***-axis determined at 77 K (1) and 300 K (2) in 3-X-C_5H_4NH-$PbBr_3$ (X = Cl, Br, I) as a function of atomic radius of the pyridine ring halogen substituent.

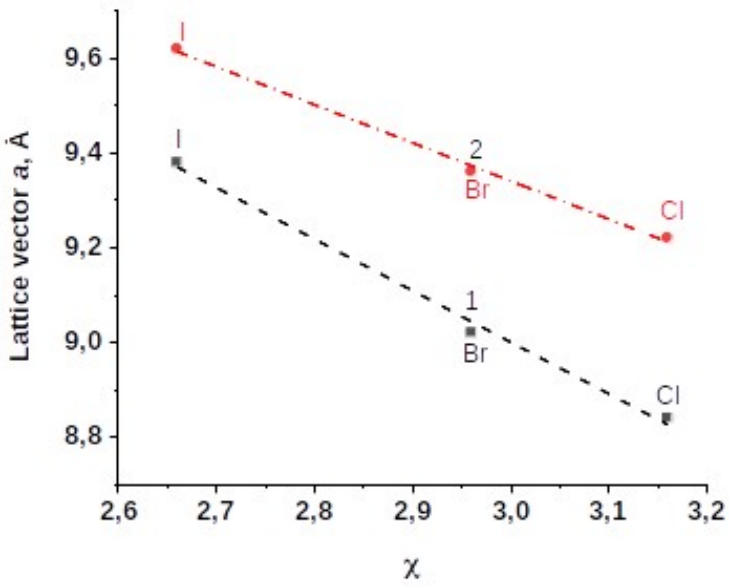

Figure S2. The length of crystallographic ***a***-axis determined at 77 K (1) and 300 K (2) in 3-X-C_5H_4NH-$PbBr_3$ (X = Cl, Br, I) as a function of electronegativity of the halogen substituent (Oganov scale [1]) in pyridine ring.

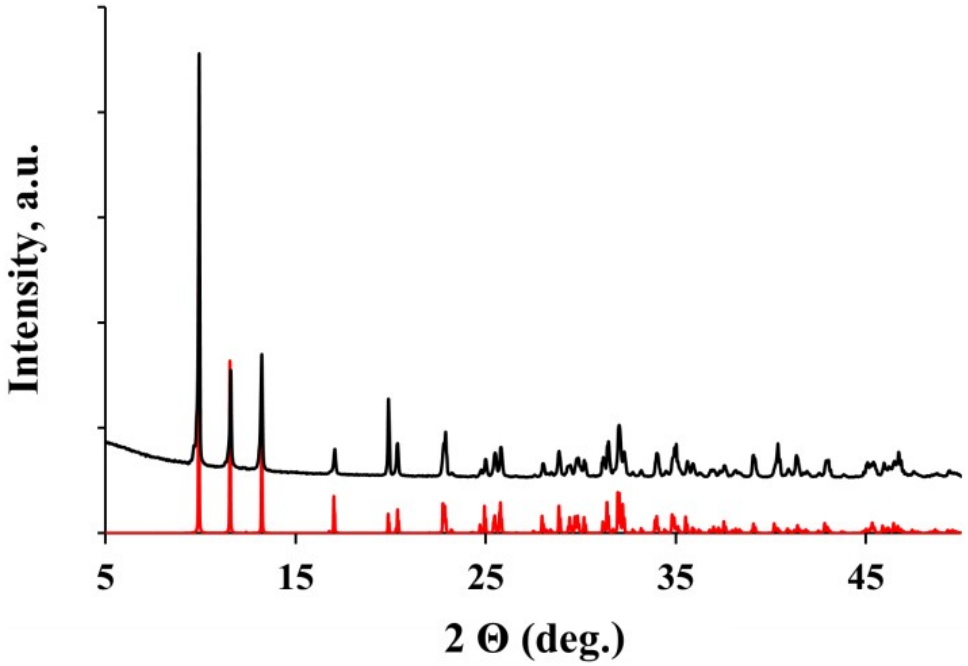

Figure S3. The experimental (black) and simulated (red) powder XRD pattern of 3-Cl-C_5H_4NH-$PbBr_3$.

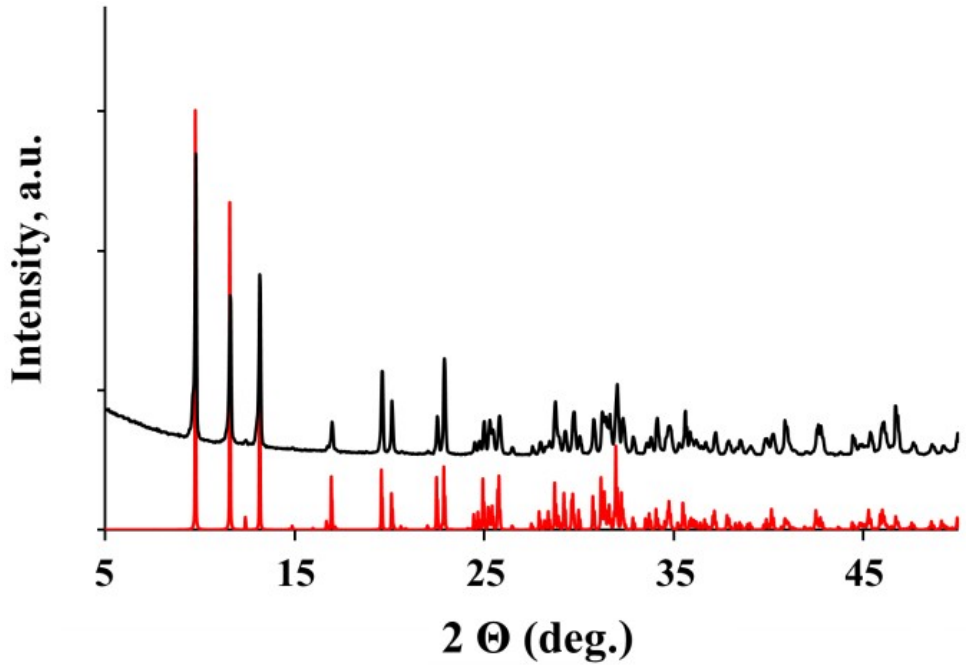

Figure S4. The experimental (black) and simulated (red) powder XRD pattern of 3-Br-C_5H_4NH-$PbBr_3$.

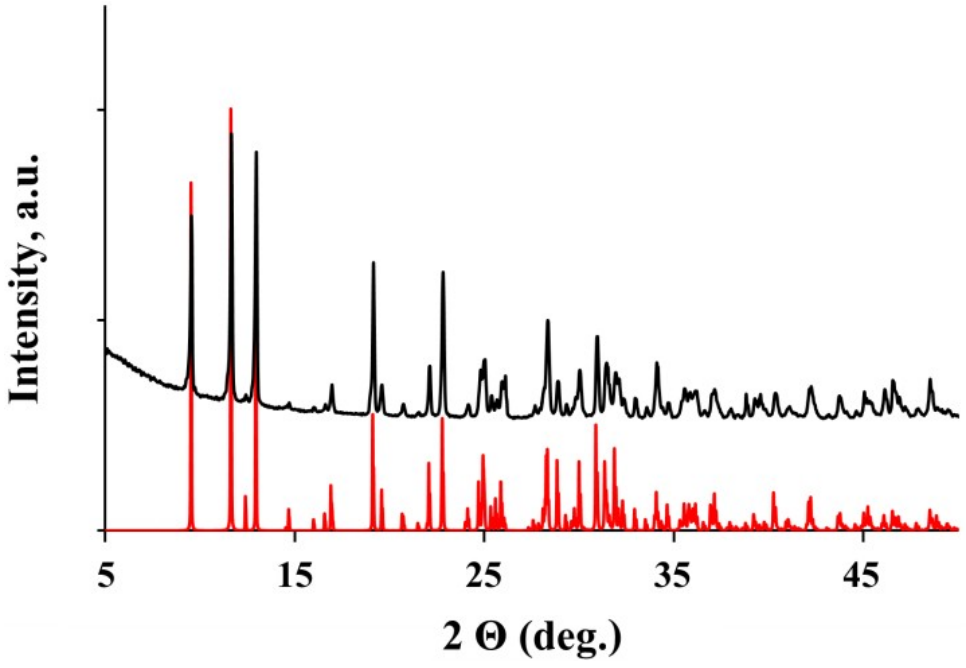

Figure S5. The experimental (black) and simulated (red) powder XRD pattern of 3-I-C_5H_4NH-$PbBr_3$.

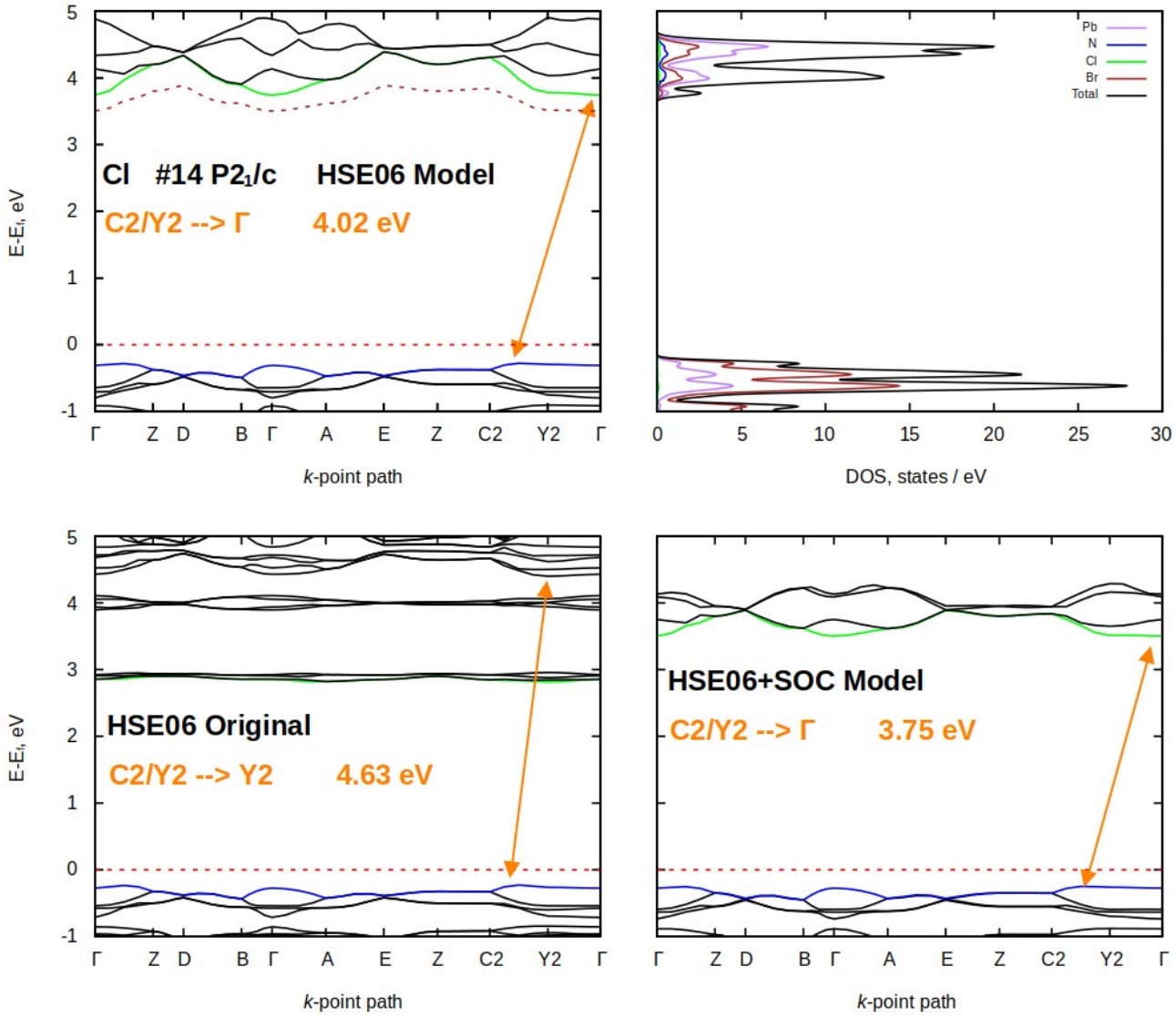

Figure S6. The upper row: HSE06 BS (left) and DOS (right) of the model chloride perovskite. The dashed brown line in the BS plot stands for the lowest energy unoccupied electronic band, computed using SOC correction. The lower row: HSE06 BS (left) and HSE06+SOC (right) of the original chloride perovskites and the model chloride perovskite, respectively. Throughout the figure the blue, green, and dashed red lines denote VB, lowest energy unoccupied electronic band, and Fermi level, respectively.

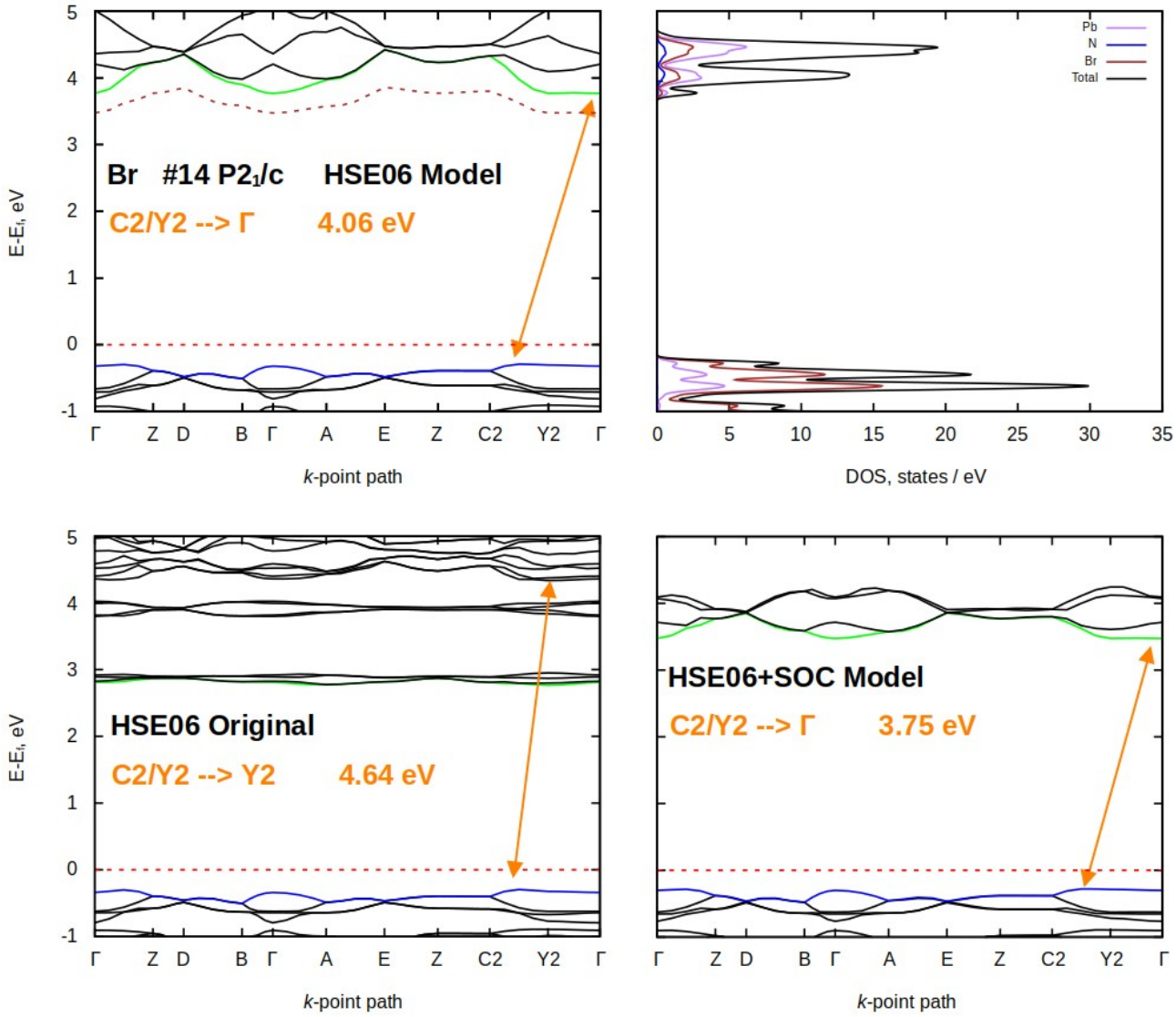

Figure S7. The upper row: HSE06 BS (left) and DOS (right) of the model bromide perovskite. The dashed brown line in the BS plot stands for the lowest energy unoccupied electronic band, computed using SOC correction. The lower row: HSE06 BS (left) and HSE06+SOC (right) of the original bromide perovskites and the model bromide perovskite, respectively. Throughout the figure the blue, green, and dashed red lines denote VB, lowest energy unoccupied electronic band, and Fermi level, respectively.

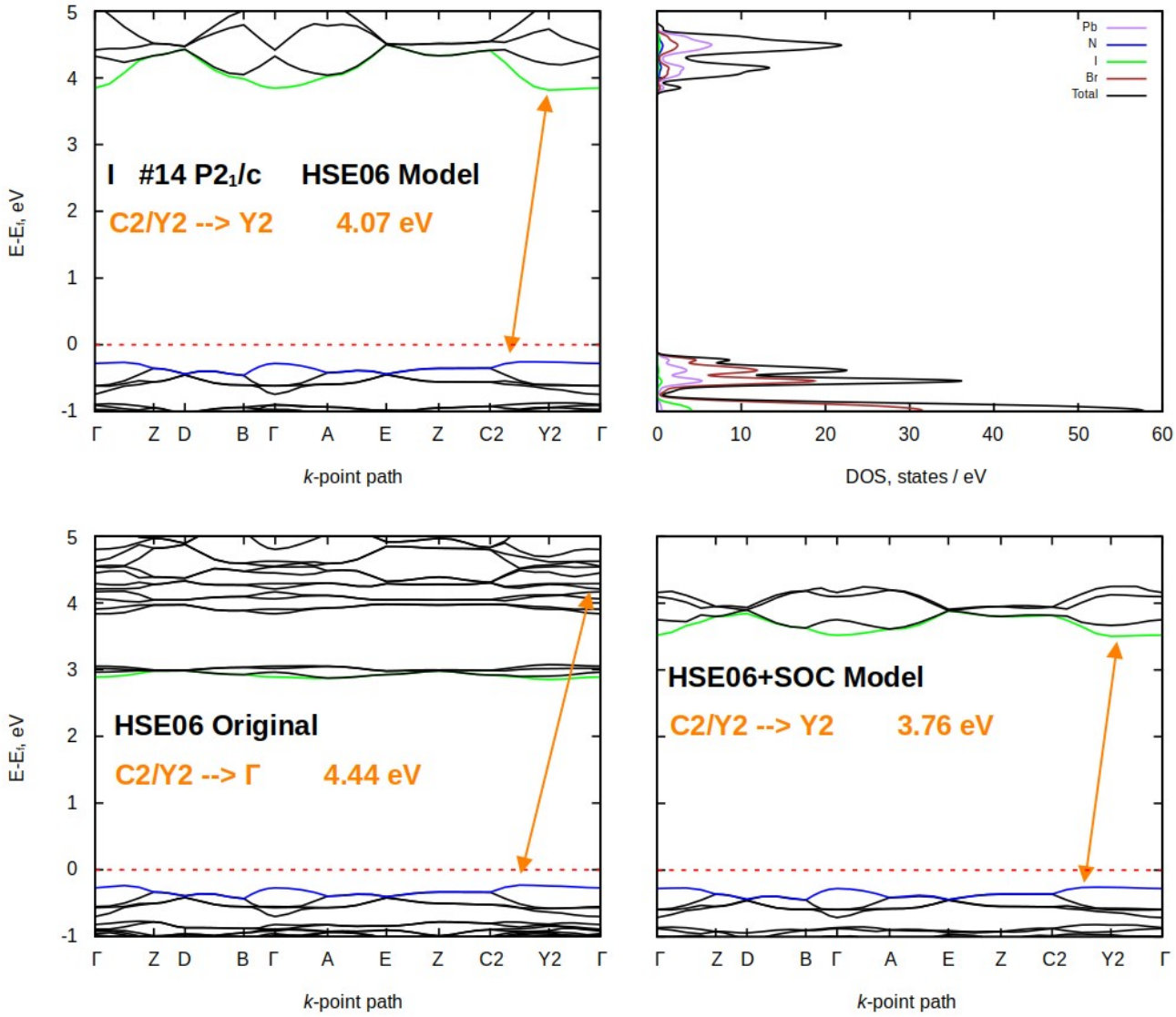

Figure S8. The upper row: HSE06 BS (left) and DOS (right) of the model iodide perovskite. The dashed brown line in the BS plot stands for the lowest energy unoccupied electronic band, computed using SOC correction. The lower row: HSE06 BS (left) and HSE06+SOC (right) of the original iodide perovskites and the model iodide perovskite, respectively. Throughout the figure the blue, green, and dashed red lines denote VB, lowest energy unoccupied electronic band, and Fermi level, respectively.

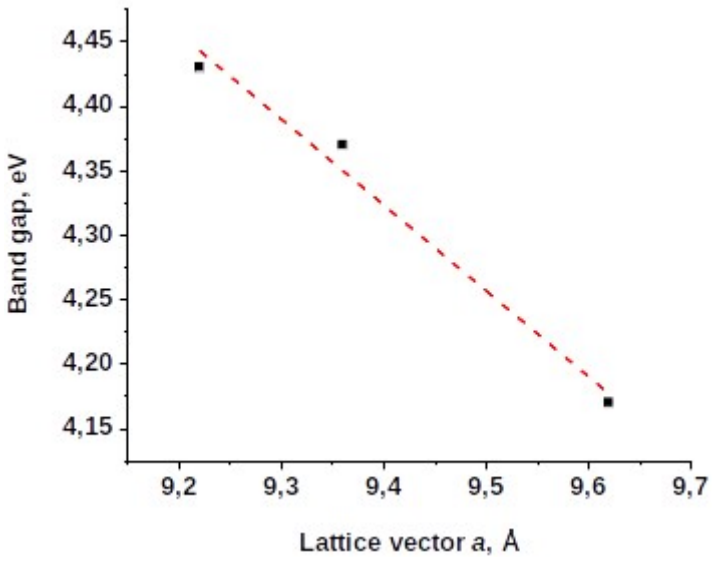

Figure S9. Correlation demonstrating a decrease of the calculated bandgap energy with elongation of the crystallographic ***a***-axes in the set of 3-X-C_5H_4NH-$PbBr_3$ (X = Cl, Br, I) structures.

1. C. Tantardini, A.R. Oganov, Thermochemical electronegativities of the elements, Nature Commun. 12 (2021) 2087, https://doi.org/10.1038/s41467-021-22429-0

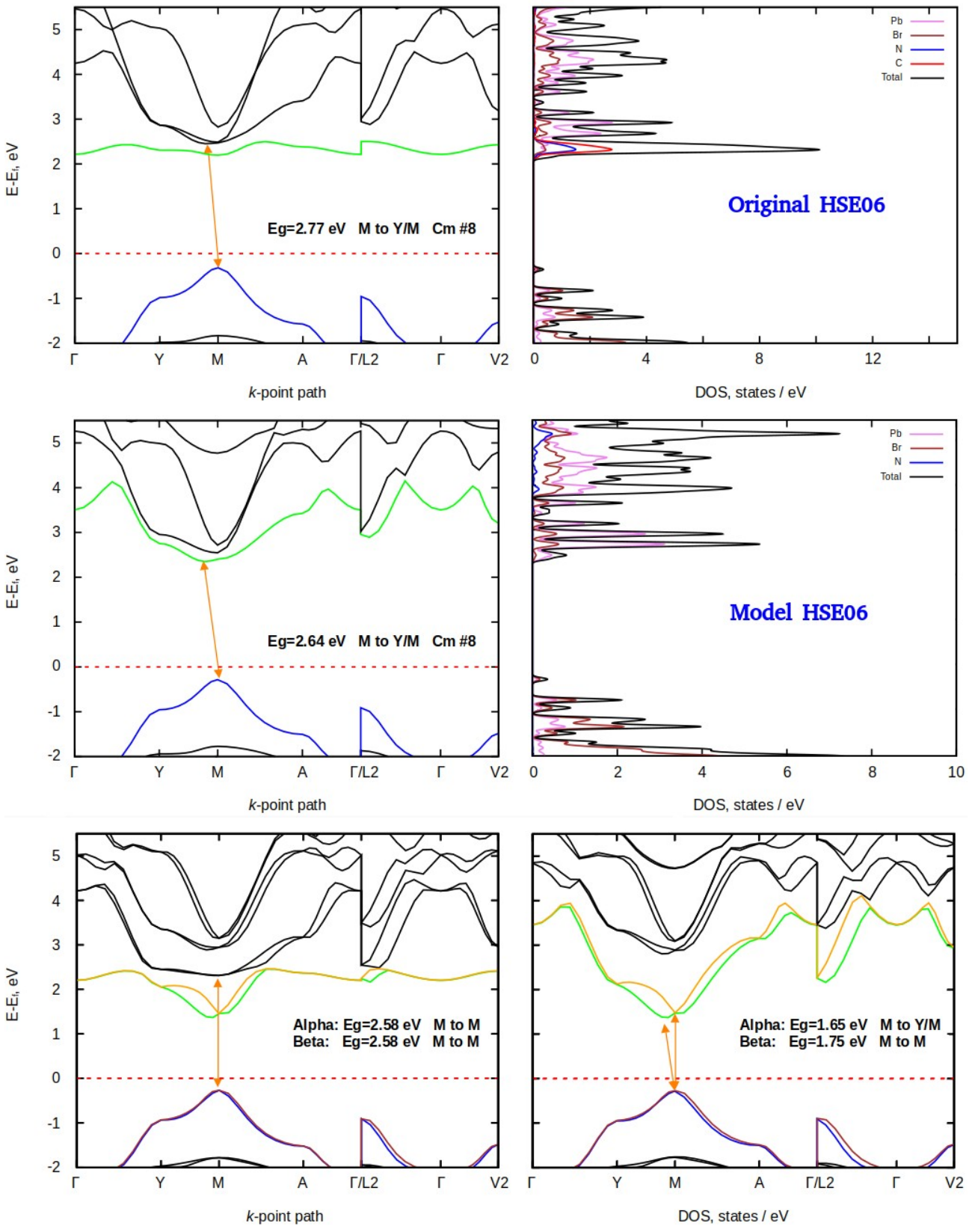

Figure S10. The upper row: HSE06 BS (left) and DOS (right) of methyleneiminium lead bromide perovskite. The middle row: HSE06 BS (left) and HSE06+DOS (right) of the model methyleneiminium lead bromide perovskite. The lower row: HSE06+SOC BS of methyleneiminium lead bromide perovskite (left) and of its model compound (right).

Throughout the figure the blue, green, and dashed red lines denote VB, lowest energy unoccupied electronic band, and Fermi level, respectively. In the lower row corresponding to SOC calculations, the brown and orange lines have the same meaning as the blue and green lines. The first and second pair of lines stands for α- and β-spin electrons, respectively.