

Engineering Halide Composition to Control Structural and Electronic Properties in Bismuth-based Perovskite-Inspired Materials

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Supporting Information

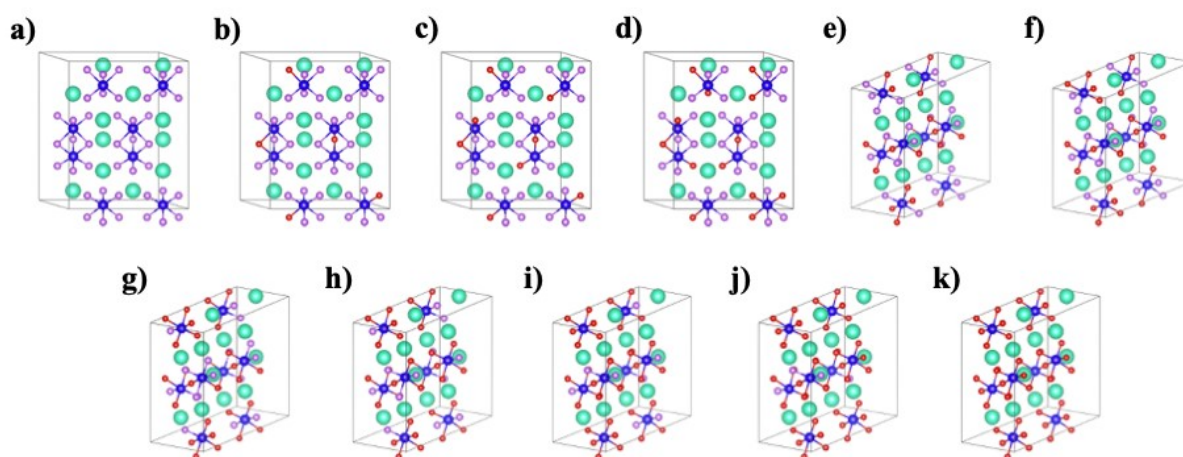


Figure S1. Optimized supercell structures of pure iodine and Br-doped compositions at various concentrations. (a) Pure iodine and Br doping levels of (b) 11%, (c) 19%, and (d) 31% in the $P6_3/mmc$ phase; and (e) 39%, (f) 50%, (g) 61%, (h) 69%, (i) 81%, (j) 89%, and (k) 100% in the $P-3m1$ phase. Color code: Bi (blue), Cs (cyan), Br (red), and I (light purple)

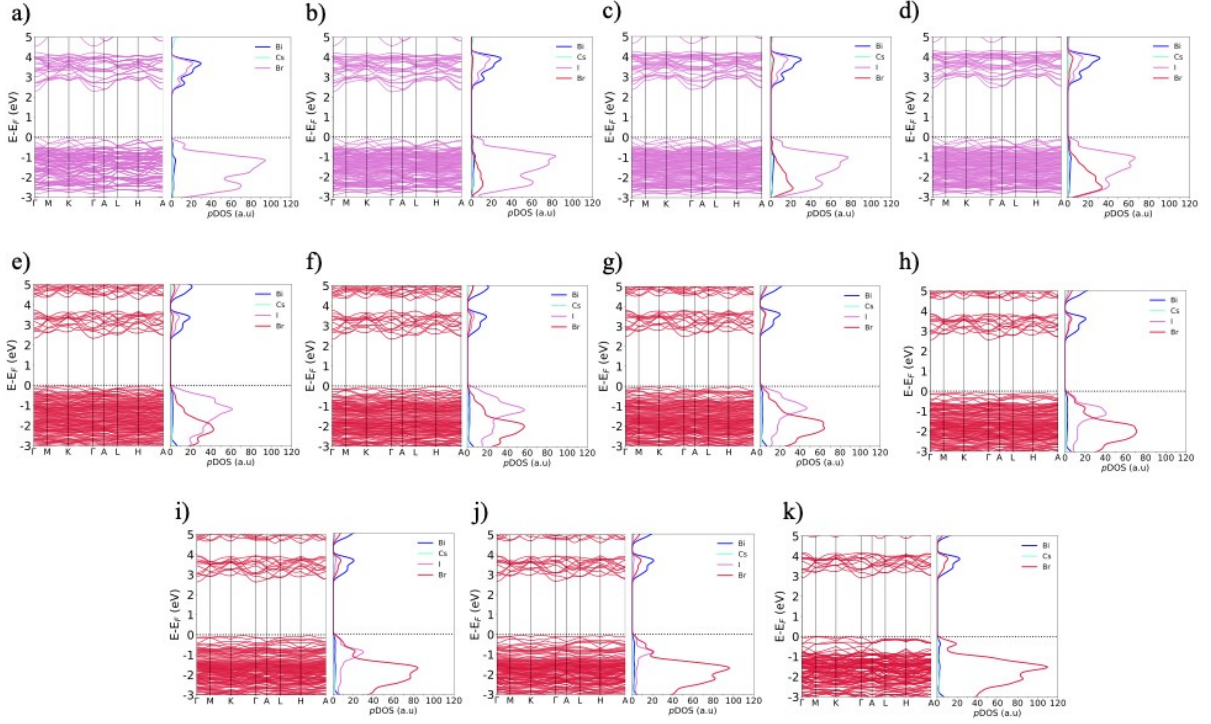


Figure S2. Electronic band structures and projected density of states (PDOS) for pure iodine and Br-doped compositions at different concentrations. (a) Pure iodine and Br doping levels of (b) 11%, (c) 19%, and (d) 31% in the $P6s/mmc$ phase; and (e) 39%, (f) 50%, (g) 61%, (h) 69%, (i) 81%, (j) 89%, and (k) 100% in the $P-3m1$ phase. Color code: Bi (blue), Cs (cyan), Br (red), and I (light purple).