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Supplemental Section

Convergence test results below are calculated using the Bi1 and Bi2 models reported in main manuscript (See Figure 5 and Table 1).

Table S0: Plane wave convergence: Column 1 includes the planewave cutoff (E_c), column 2 is the Bi1model total energy (E_{Bi1}^{tot}), column 3 is the Bi2 total energy (E_{Bi2}^{tot}), column 4 is the energy difference $\Delta E = E_{Bi2}^{tot} - E_{Bi1}^{tot}$, column 5 is$\Delta E$ per number of $CuBiI_4$formula units, column 6 and 7 are the Bi1 and Bi2 band gaps(E_{gap}^{Bi1}, E_{gap}^{Bi2}), respectively. As illustrated, the physical properties of interest ΔE per f.u. and the band gap values are converged to within 0.01 eV for $E_c = 250\ eV$.

1	2	3	4	5	6	7
$E_c(eV)$	$E_{Bi1}^{tot}(eV)$	$E_{Bi2}^{tot}(eV)$	$\Delta E\ (eV)$	$\Delta E\ per\ f.u.(eV)$	$E_{gap}^{Bi1}(eV)$	$E_{gap}^{Bi2}(eV)$
175	−99.261	−96.800	2.461	0.308	1.792	1.913
250	−113.012	−112.515	0.497	0.062	1.533	1.574
325	−113.208	−112.657	0.551	0.069	1.518	1.553
400	−113.169	−112.622	0.547	0.068	1.523	1.557
475	−113.198	−112.648	0.550	0.069	1.523	1.563

Table S1: K-point convergence allowing the atoms to relax for each K-point grid while keeping the lattice vectors fixed. The plane wave cutoff is $E_c = 400\ eV$ for each calculation. Column 1 includes the K-grid integers (Kpt), column 2 is the Bi1 model total energy (E_{Bi1}^{tot}), column 3 is the Bi2 total energy (E_{Bi2}^{tot}), column 4 is the energy difference $\Delta E = E_{Bi2}^{tot} - E_{Bi1}^{tot}$, column 5 is ΔE per number of $CuBiI_4$ formula units. As illustrated, the physical property of interest ΔE per f.u. are converged to within 0.001 eV for Γ calculations.

1	2	3	4	5
$Kpts$	$E_{Bi1}^{tot}(eV)$	$E_{Bi2}^{tot}(eV)$	$\Delta E^{tot}(eV)$	$\Delta E\ per\ f.u.(eV)$
$1x1x1$	−113.169	−112.622	0.547	0.068
$2x2x2$	−113.776	−113.218	0.542	0.069
$3x3x3$	−113.774	−113.221	0.553	0.069

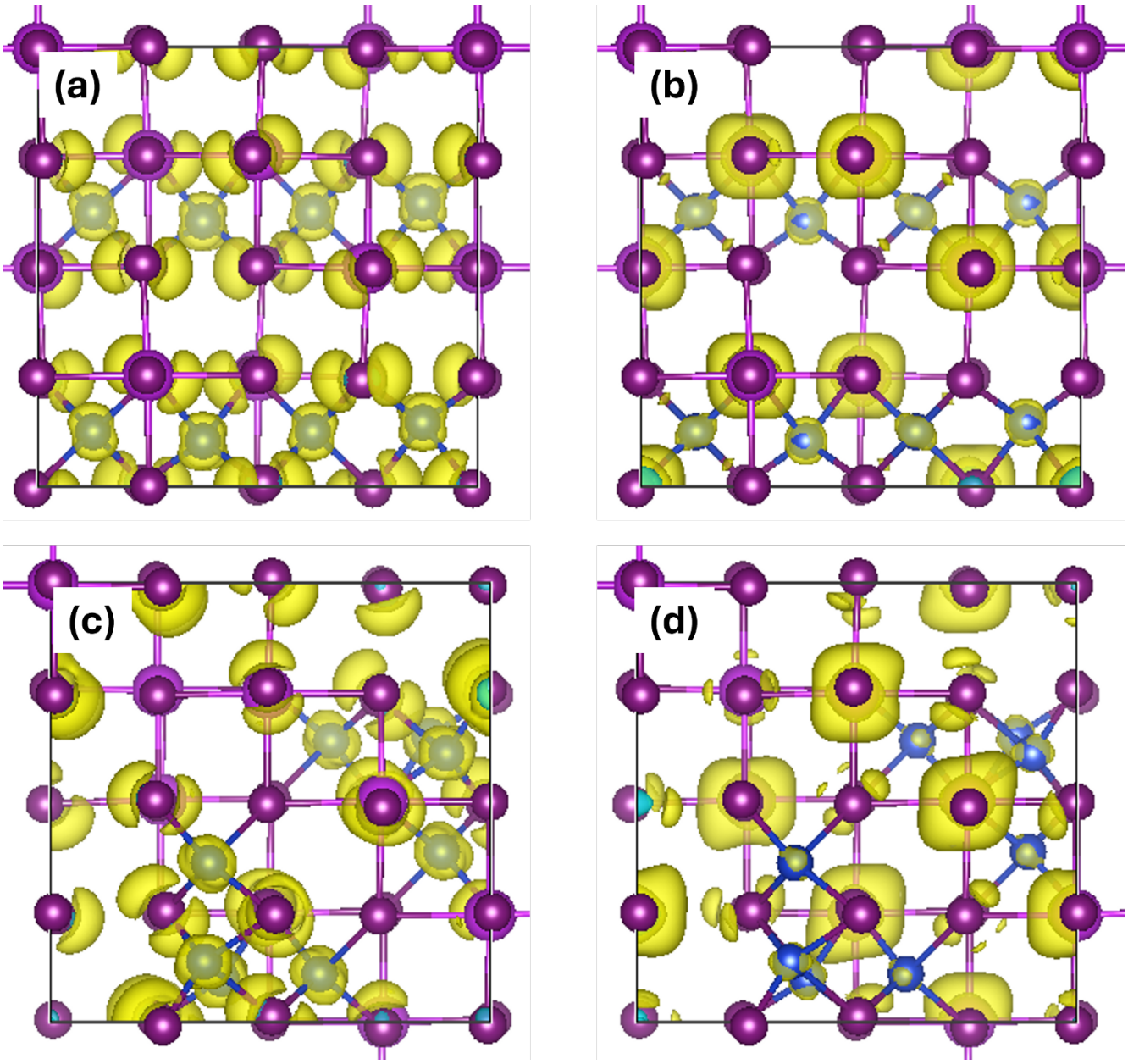

Figure S1: The ball-and-stick image of the band edge states for the Bi1 and Bi2 models. Specifically, (a)Bi1 valence band states, (b) Bi1 conduction band states, (c) Bi2 valence band states and (d) Bi2 conduction band states. The yellow regions show iso-surfaces of constant band state density $|\psi^2|$.

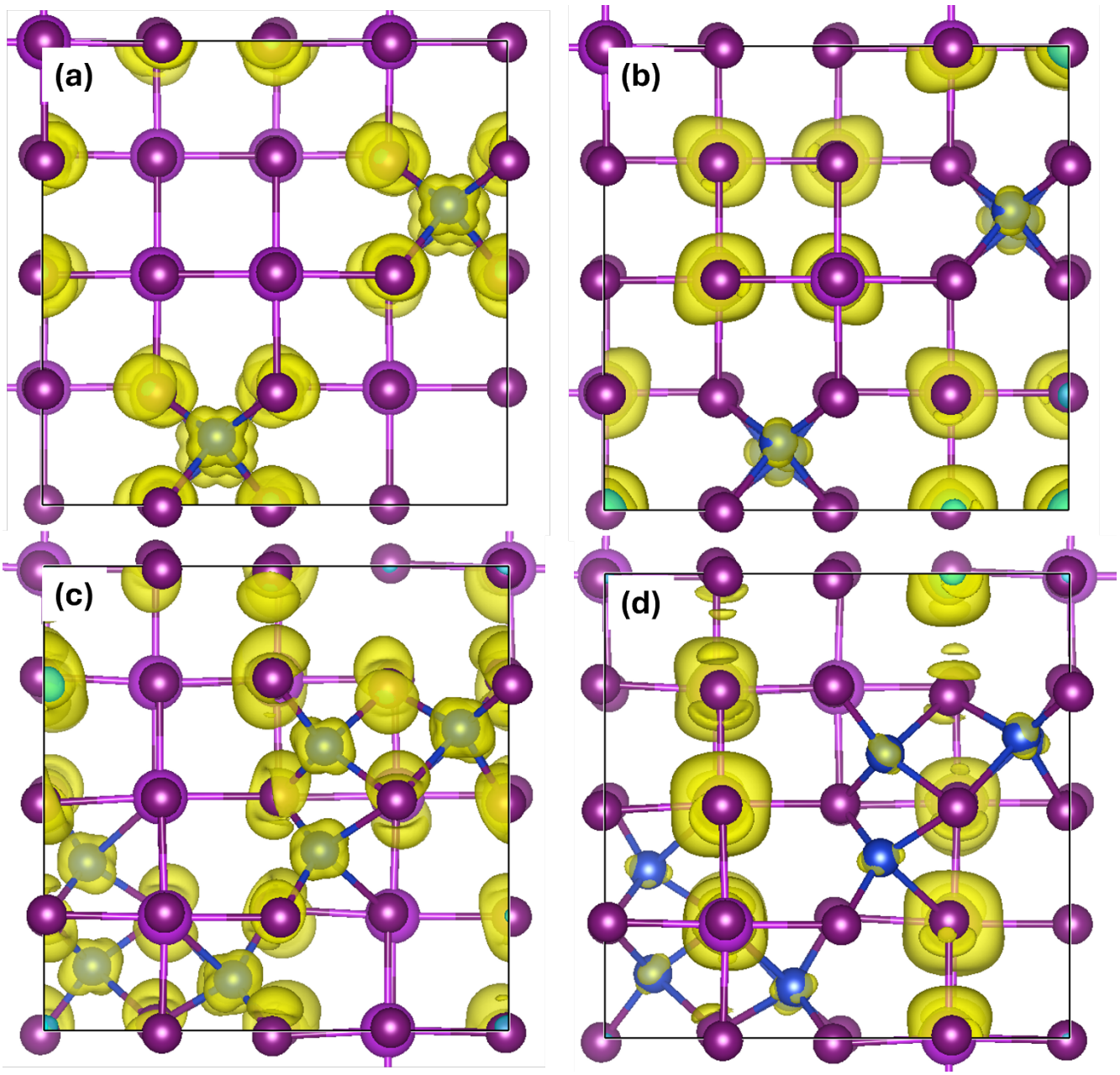

Figure S2: Same as Figure S1 but rotated by 90 degrees. The ball-and-stick image of the band edge states for the Bi1 and Bi2 models. Specifically, (a)Bi1 valence band states, (b) Bi1 conduction band states, (c) Bi2 valence band states and (d) Bi2 conduction band states. The yellow regions show iso-surfaces of constant band state density $|\psi^2|$.

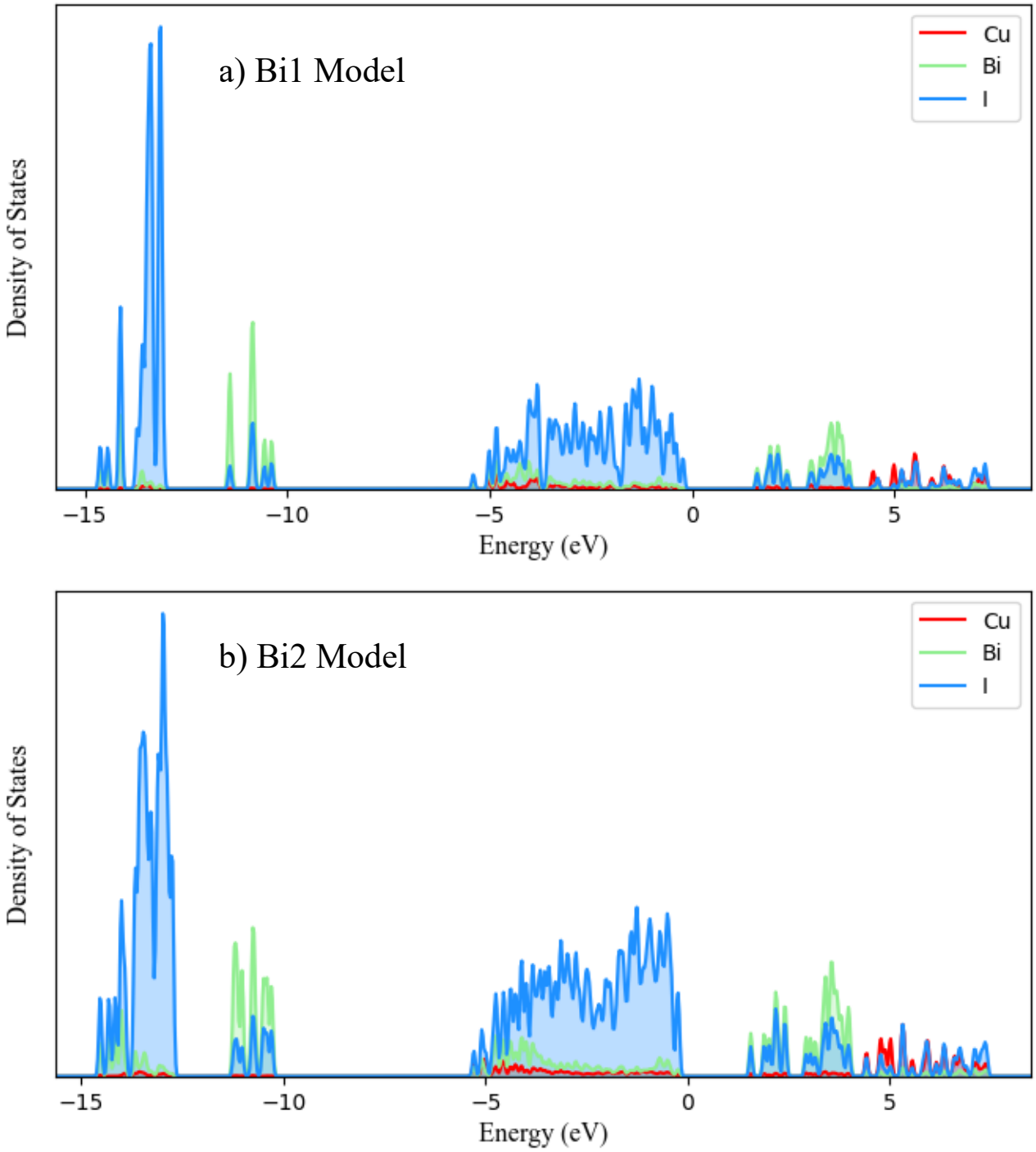

Figure S3: The full density of states plots for the a) Bi1 model and b) Bi2 model.