

## SUPPORTING INFORMATION

### Ab initio X-ray Near-Edge Spectroscopy of Sodium-Based Multi-Alkali Antimonides

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TABLE S1. Number of degenerate excitons below the onset computed in the independent-particle approximation with their binding energies in meV.

	cNa <sub>2</sub> KSb		cNaK <sub>2</sub> Sb		hNa <sub>2</sub> KSb		hNaK <sub>2</sub> Sb	
	# excitons	$E_b$						
Na K-edge	2	229	2	574	2	70	2	131
	2	59	2	55				
K K-edge	2	111	2	66	2	60	2	125
K L <sub>2,3</sub> -edge	4	112	4	66	4	61	4	126
Sb K-edge	2	105	2	66	2	59	2	120
Sb L <sub>2</sub> -edge	2	108	2	68	2	61	2	124

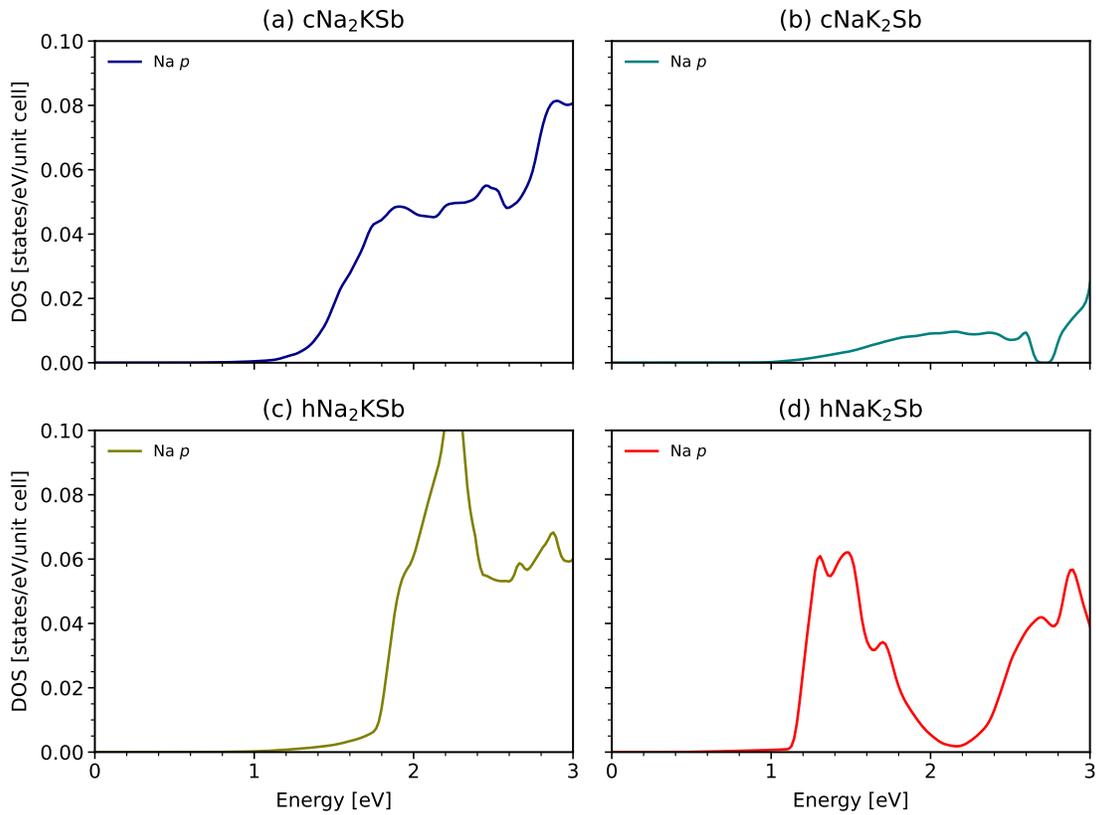


FIG. S1. Contribution of Na  $p$ -states to the lowest-energy unoccupied density of states of (a) cNa<sub>2</sub>KSb, (b) NaK<sub>2</sub>Sb, (c) hNa<sub>2</sub>KSb, and (d) hNaK<sub>2</sub>Sb, with the conduction band minimum set at 0 eV.

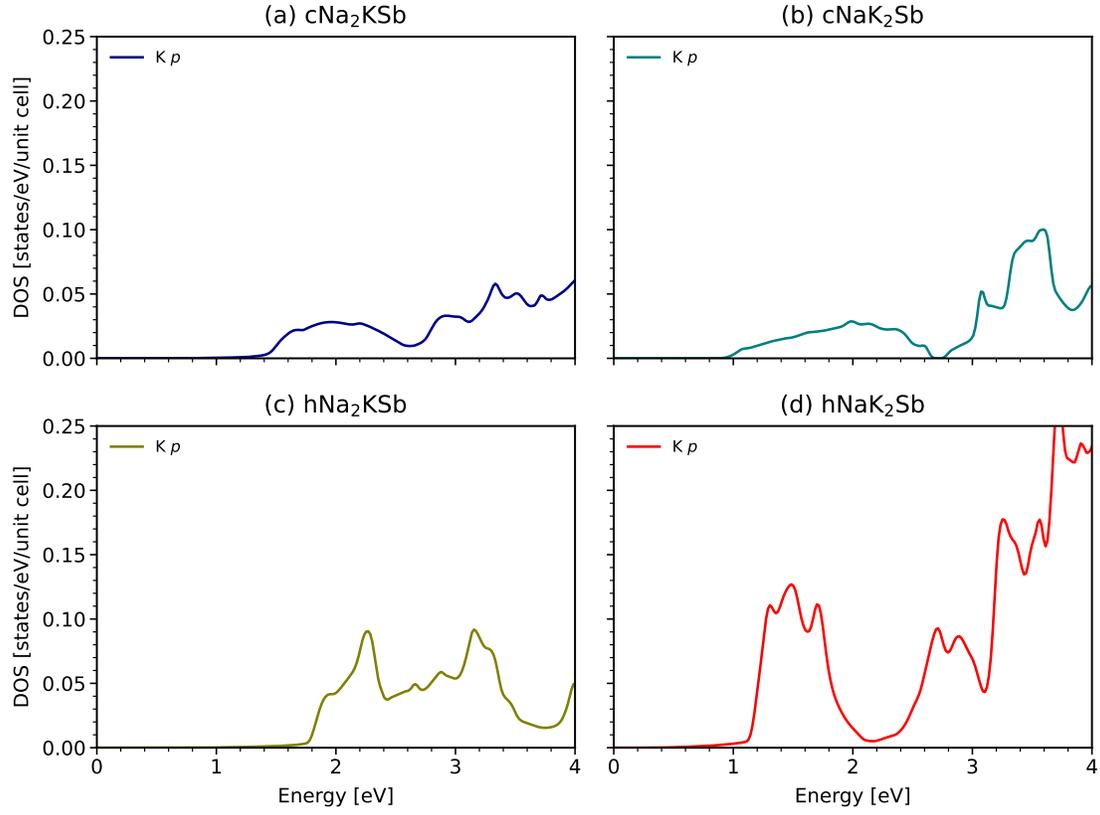


FIG. S2. Contribution of K  $p$ -states to the lowest-energy unoccupied density of states of (a)  $c\text{Na}_2\text{KSb}$ , (b)  $\text{NaK}_2\text{Sb}$ , (c)  $h\text{Na}_2\text{KSb}$ , and (d)  $h\text{NaK}_2\text{Sb}$ , with the conduction band minimum set at 0 eV.

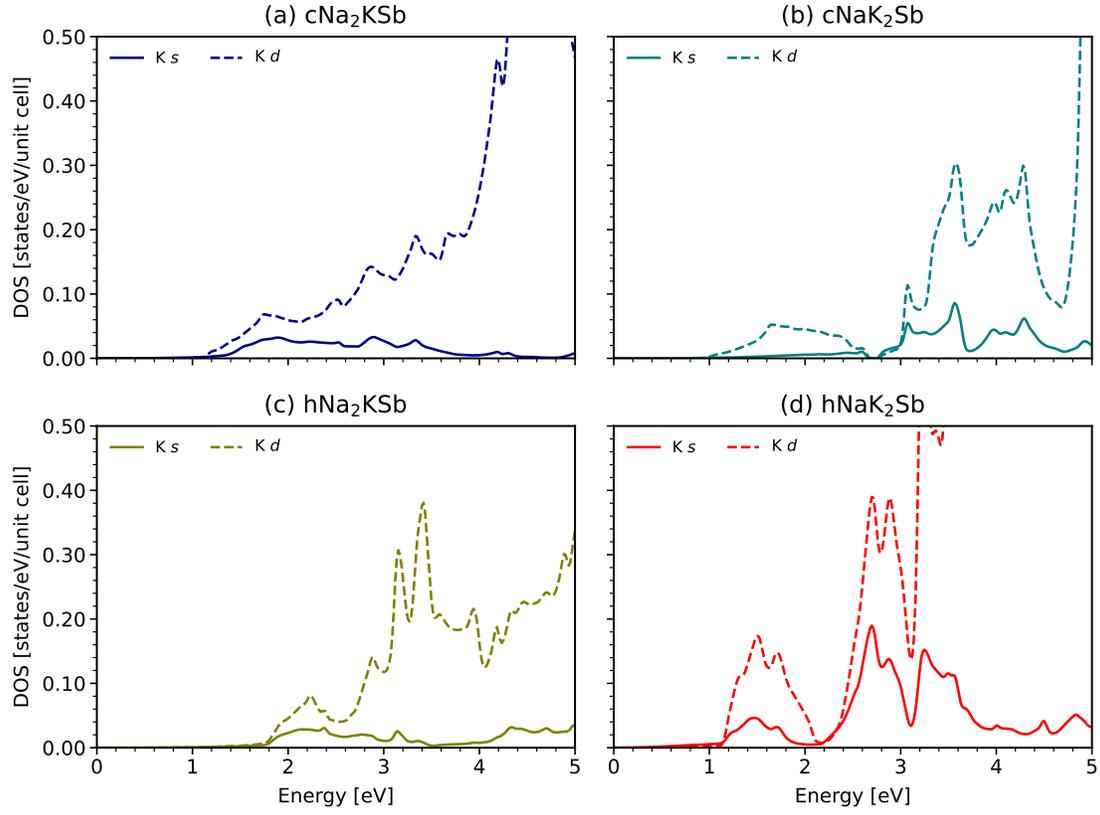


FIG. S3. Contributions of K *s*-states (solid lines) and K *d*-states (dashed lines) to the lowest-energy unoccupied density of states of (a)  $c\text{Na}_2\text{KSb}$ , (b)  $\text{NaK}_2\text{Sb}$ , (c)  $h\text{Na}_2\text{KSb}$ , and (d)  $h\text{NaK}_2\text{Sb}$ , with the conduction band minimum set at 0 eV.

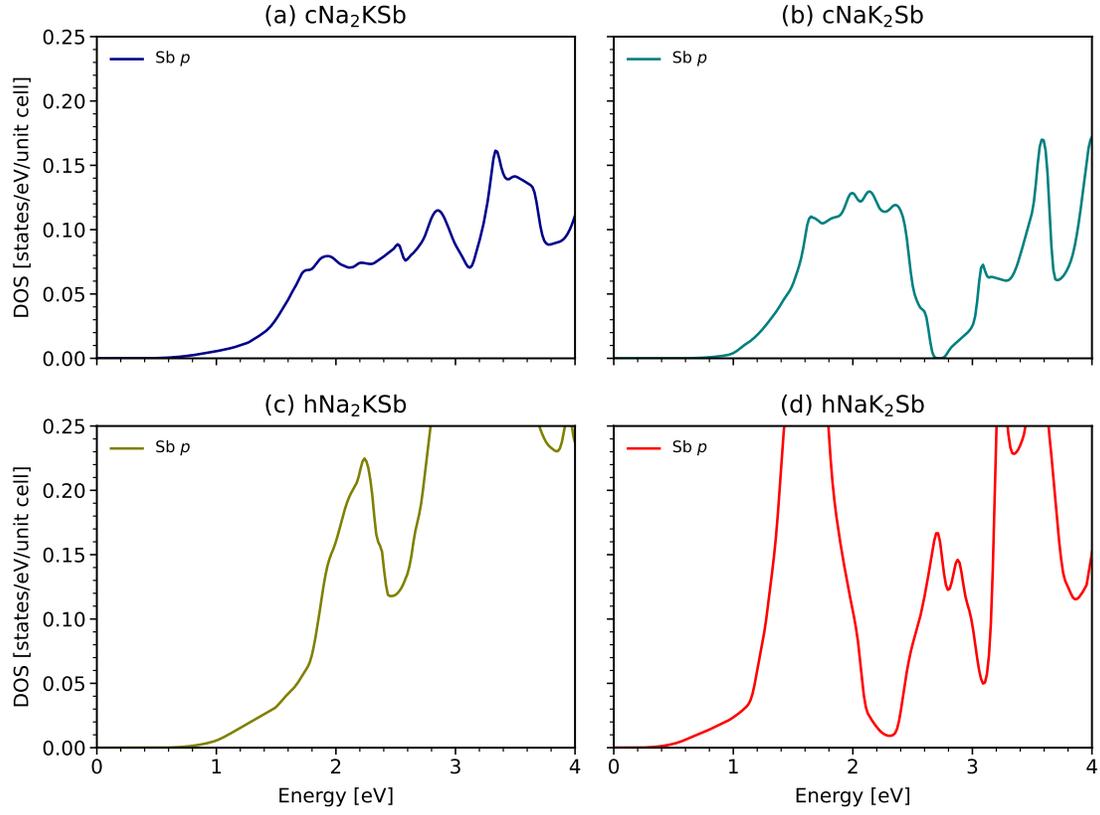


FIG. S4. Contribution of Sb  $p$ -states to the lowest-energy unoccupied density of states of (a)  $c\text{Na}_2\text{KSb}$ , (b)  $\text{NaK}_2\text{Sb}$ , (c)  $h\text{Na}_2\text{KSb}$ , and (d)  $h\text{NaK}_2\text{Sb}$ , with the conduction band minimum set at 0 eV.

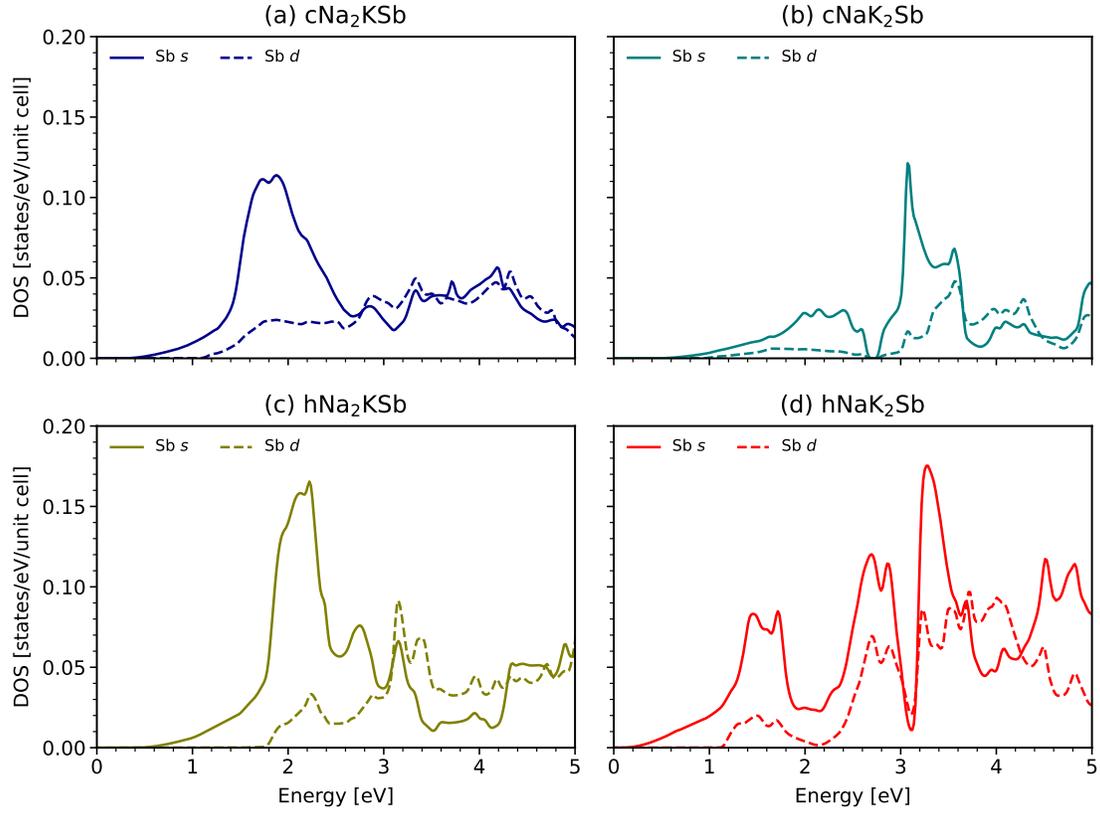


FIG. S5. Contributions of Sb *s*-states (solid lines) and Sb *d*-states (dashed lines) to the lowest-energy unoccupied density of states of (a)  $c\text{Na}_2\text{KSb}$ , (b)  $\text{NaK}_2\text{Sb}$ , (c)  $h\text{Na}_2\text{KSb}$ , and (d)  $h\text{NaK}_2\text{Sb}$ , with the conduction band minimum set at 0 eV.