Theoretical prediction of O-B_2S_2 monolayer as two-dimensional sodium-ion battery anode material by first-principles calculations

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Compositional convex hull of the B-S-O chemical system constructed from Materials Projectreference data. Stable phases forming the convex hull are indicated by solid symbols. The proposed B_2S_2O phase (this work) is highlighted in red and is located above the convexhull, indicating thermodynamic metastability with respect to decomposition into B_2O_3, BS_2, and S.

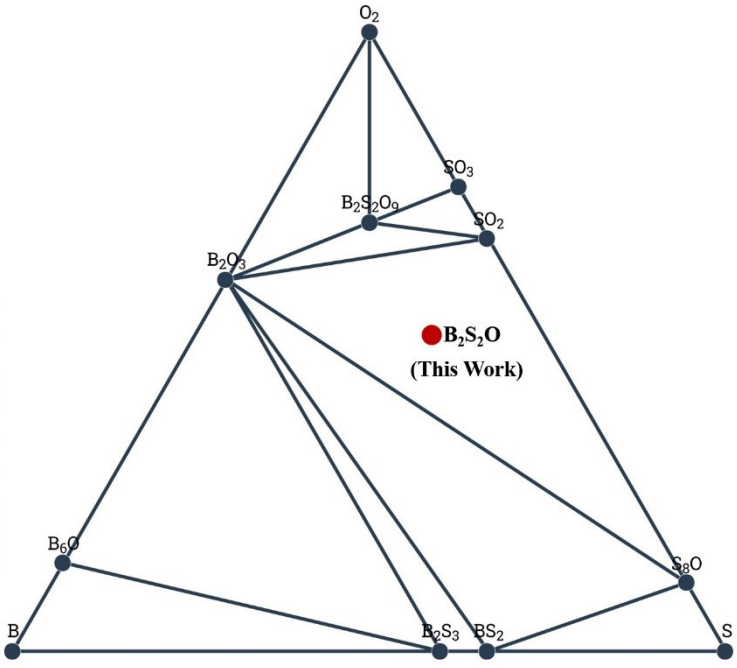

Fig. S1 Convex-hull analysis illustrating the thermodynamic metastability of B2S2O in the ternary B-S-O chemical system.

Normalized formation energies of representative Na adsorption configurations as a function of Na content x in Na_x–O–B_2S_2. The energies are normalized such that the endpoints at x = 0 and x = 24 are set to zero to

emphasize the relative stability trend upon Na insertion. Purple symbols denote the energies of representative optimized configurations at each Na concentration, while the blue solid line connects the lowest-energy configurations and serves as an approximate lower convex hull. This construction is used to illustrate the energetic landscape underlying the voltage profile, rather than a fully exhaustive enumeration of all possible Na orderings.

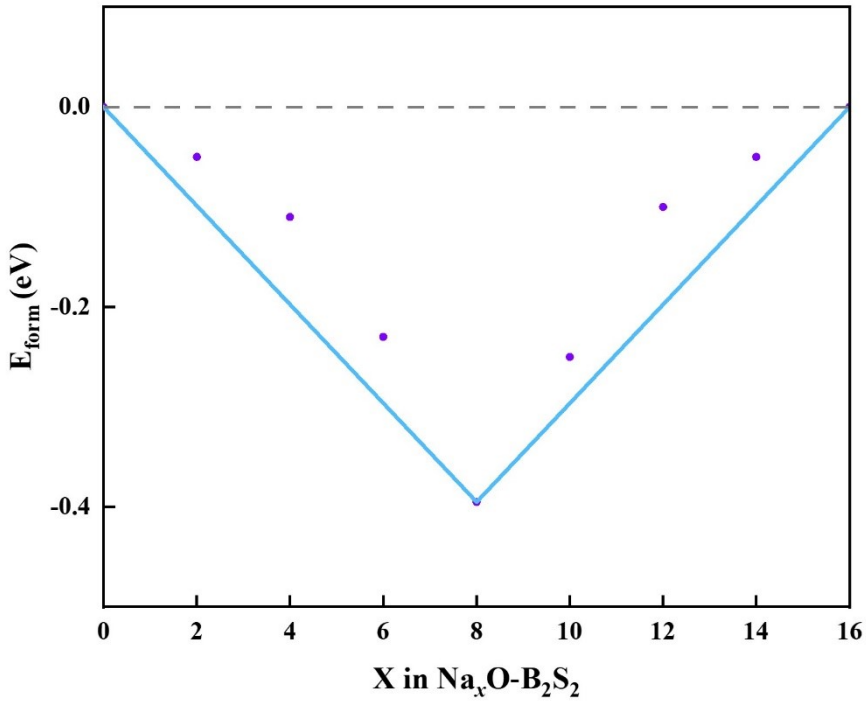

Fig. S2 Normalized formation-energy landscape and approximate convex hull of Na_x–O–B_2S_2.

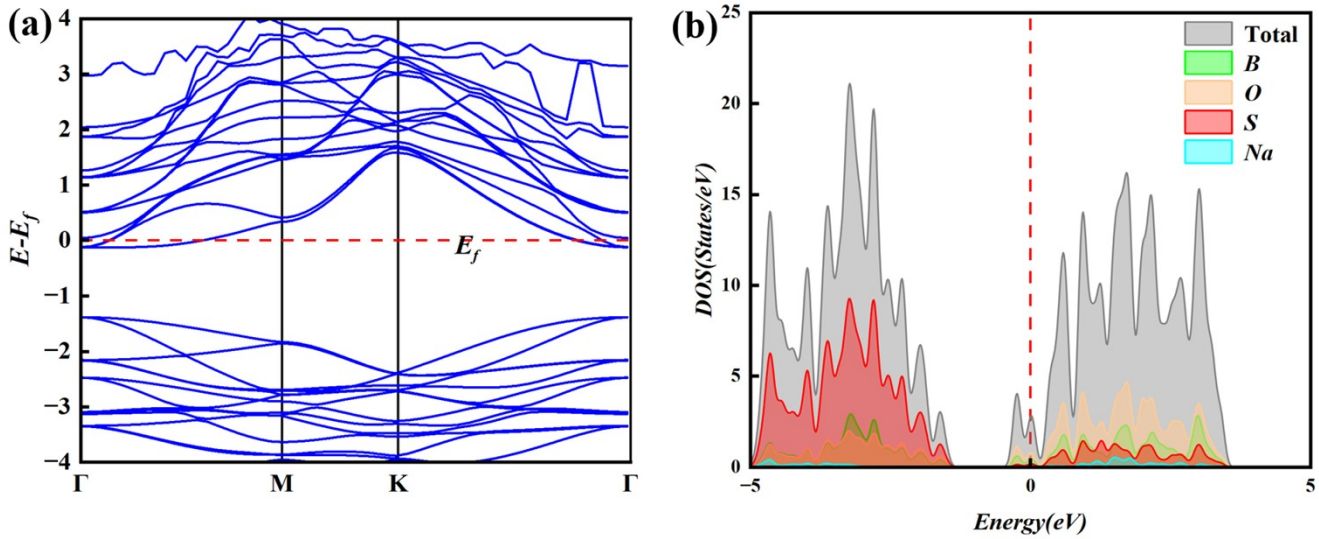

Fig. S3 (a) Electronic band structure of the O-B_2S_2 monolayer with a single Na atom adsorbed at the most stable Hollow site, calculated at the PBE level along the Γ–M–K–Γ path. (b) Corresponding total DOS, showing finite electronic states at the Fermi level (set to zero), indicating metallic behavior upon Na adsorption.

Thermodynamically stable phases (hull vertices) in the B-S-O chemical system obtained from the Materials Project database. The listed values correspond to formation energies per atom (relative to elemental reference states) reported by Materials Project, and the MP identifiers (MP id) are provided to enable reproducible reconstruction of the B-S-O convex hull used in this work.

Table S1. Thermodynamically stable phases forming the B-S-O convex hull (Materials Project reference data) used for the stability assessment of B_2S_2O.

Stable phase	formation energy (eV/atom)	MP id
B	0	mp-160
B_2O_3	-2.798	mp-306
$B_2S_2O_9$	-2.166	mp-1019509
B_2S_3	-0.735	mp-1199451
B_6O	-0.805	mp-1346
BS_2	-0.73	mp-540668
O_2	0	mp-12957
S	0	mp-96
S_8O	-0.644	mp-27465
SO_2	-1.69	mp-27726
SO_3	-1.703	mp-2414

Table S2. In-plane lattice variation of O-B_2S_2 upon Na adsorption

Na loading	a (Å)	b (Å)	γ(Å)	Area change (%)
0 Na (pristine)	6.17866	6.17863	120.00	0
16 Na (high coverage)	6.59644	6.59435	120.01	~13.9