Supplementary Information for

Potassium cation storage and diffusion in SnS, SnS_2, and at SnS/SnS_2 interfaces

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Structures of relaxed systems before adding K^+ ions

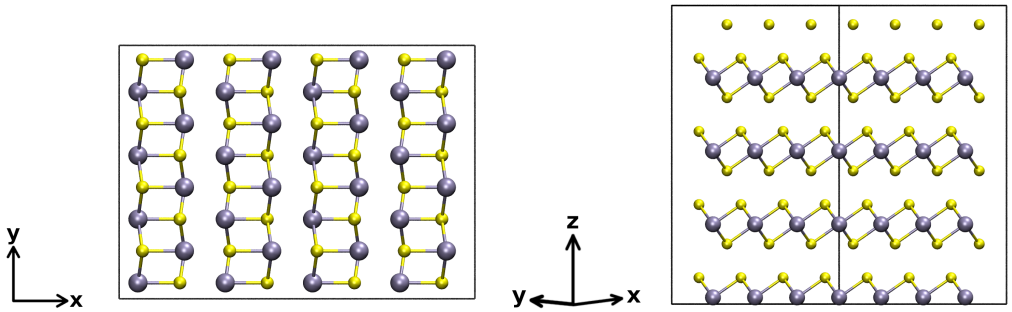

Figure 1: Relaxed structures of bulk SnS (left) and SnS_2 (right) considered in this work. Tin atoms are shown in gray, sulfur atoms in yellow.

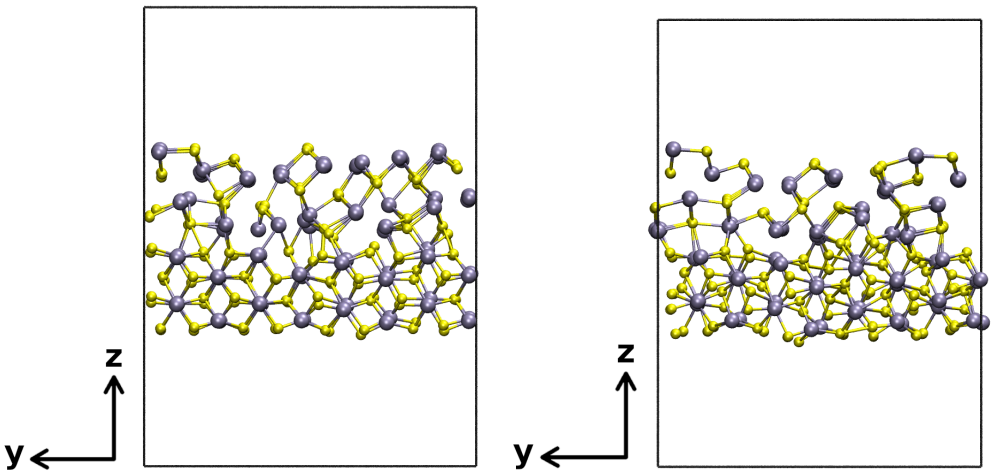

Figure 2: Relaxed SnS/SnS_2 interfaces formed by a (302) surface slab of SnS and a (110) surface slab of SnS_2 with two different terminations, labeled as interface 1a (left) and interface 1b (right).

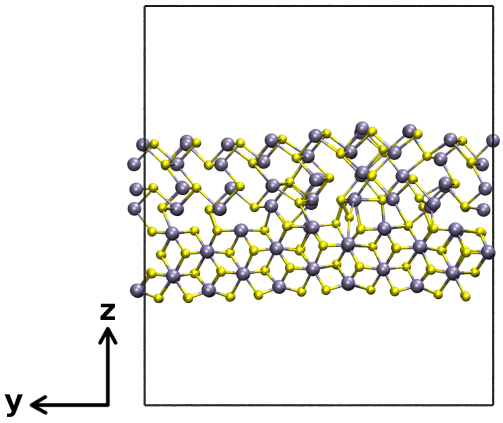

Figure 3: Relaxed SnS/SnS_2 interface formed by a (020) surface slab of SnS and a (110) surface slab of SnS_2, labeled as interface 2.