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Computational study of ideal electrolyte/anode interfaces for Na3SbS4/Na[1] LARRY E. RUSH JR., N.A.W. HOLZWARTH, Wake Forest University — As part of an effort to develop energy storage technology based on Na-ion batteries, recent papers in the literature[2] demonstrate the electrochemical stability of the solid electrolyte Na_3SbS_4 interfaced with a metallic Na anode. The integrity of this electrolyte/anode interface, which is essential to the success of these battery components, is attributed to the formation of a stable solid-electrolyte interphase (SSEI). We report the results of a computational study of this system, using first-principles methods to model ideal interfaces of Na_3SbS_4 with Na metal. The ideal interfaces were constructed from (110), (100), and (001) surfaces of tetragonal crystals of Na_3SbS_4 and Na metal in various configurations. The results show several likely components of the SSEI including a few broken Sb−S bonds and Na_2S groups stabilized at the outer layer of the interface.

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[2]Wang *et al.*, **Angew. Chem. Int. Ed. 55**, 85518555 (2016), Zhang *et al.*, **Adv. Sci. 2016**, 1600089 (2016)

Larry E. Rush Jr.
Wake Forest University

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