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First-principles calculations of barium hydride for hydrogen transport applications[1] ANDREW ROWBERG, LEIGH WESTON, CHRIS G. VAN DE WALLE, Materials Department, University of California, Santa Barbara — Barium hydride is one of several thermally stable alkaline earth hydrides (AeH_2; Ae = Sr, Ca, Ba) to hold potential interest for future hydrogen transport applications, based on its high conductivity of hydride ions over a broad temperature range. However, the underlying materials processes at play in promoting this conductivity remain to be elucidated. A greater understanding of the mechanisms enabling efficient hydride ion migration within BaH_2 is needed to move the material closer to applications. Toward that end, we conduct first-principles calculations based on density functional theory with a hybrid functional. We characterize the bulk electronic and structural properties of BaH_2 and study the mechanism of hydride ion migration and the influence of native point defects on ionic conductivity.

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