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Barium disilicides ($BaSi_2$) a low-cost, earth-abundant material for thin-film solar cells MUKESH KUMAR, NAOTO UMEZAWA, MOTOHARU IMAI, Natl Inst for Materials Sci — In order to meet the clean energy requirement, materials consisting of abundant, eco-friendly, and low-cost elements are of great interest. Therefore in this study, we discussed the importance of $BaSi_2$ and other similar semiconducting compounds which contain inexpensive and earth abundant elements, for solar cell applications. Employing first-principles modeling within the density function theory, we analyze the structural, electronic and optical properties and find that these compounds have fundamental indirect band gaps and the gap energies are in the region of 0.9–1.3 eV, which is suitable for solar cell applications. Furthermore, a lower energy dispersion of the conduction band (CB), which results in a flat shape of the CB minimum, implies a large optical absorption. In fact, our calculations reveal that the photoabsorption of these compounds is stronger than other common PV materials like Si and $Cu(Ga,In)Se_2$.

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