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Properties of the chalcogenide-based double perovskites Ba_2NbBiS_6 and Ba_2TaSbS_6 with respect to structural, electronic and optical aspects

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In this work, we delve into the investigation of the structural, electronic, and optical properties of Ba_2NbBiS_6 and Ba_2TaSbS_6 chalcogenide-based double perovskites, which are structured in the cubic space group $Fm\bar{3}m$ form. We have performed first-principles calculations using density functional theory (DFT) to study the above properties. The electronic band structure and density of states of this compound have been investigated, and their results show that Ba_2NbBiS_6 and Ba_2TaSbS_6 exhibit a semiconducting nature with an indirect energy gap of 1.680 eV and 1.529 eV, respectively. Furthermore, an investigation was conducted on the optical properties of the compounds throughout the energy range spanning from 0 eV to 55 eV. This investigation focused on many parameters, including dielectric functions, optical reflectivity, refractive index, extinction coefficient, optical conductivity, and electron energy loss. The optical data obtained from the calculations reveals that all compounds demonstrate isotropy in optical polarization. Furthermore, it has been noted that our compounds exhibit absorption properties inside the ultraviolet (UV) region. Consequently, these materials hold promise as potential candidates for various applications, such as UV photodetectors, UV light emitters, and power electronics. This is primarily attributed to their inherent absorption limits and the presence of prominent absorption peaks in this spectral range. In brief, chemical mutation techniques have been employed to manipulate the characteristics of double-sulfide perovskites to develop durable and environmentally friendly perovskite materials suitable for solar purposes.

Keywords: DFT; optoelectronics; chalcogenide double perovskites; optical properties.

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