First-principles calculations of structural, elastic, electronic, and optical properties of perovskite-type KMgH3 crystals: Novel hydrogen storage material

Abstract

We report a first-principles study of structural and phase stability in three different structures of perovskite-types KMgH3 according to H position. While electronic and optical properties were measured only for stable perovskite-type KMgH3, our calculated structural parameters are found in good agreement with experiment and other theoretical results. We also study the electronic charge density space distribution contours in the (200), (101), and (100) crystallographic planes, which gives better insight picture of chemical bonding between K-H, K-Mg-H, and Mg-H. Moreover, we have calculated the electronic band structure dispersion, total, and partial density of electron states to study the band gap origin and the contribution of s-band of H, s and p-band of Mg in the valence band, and d-band of K in the conduction band. Furthermore, optical features such as dielectric functions, refractive indices, extinction coefficient, optical reflectivity, absorption coefficients, optical conductivities, and loss functions of stable KMgH3 were calculated for photon energies up to 40 eV.