First principles study of electronic structure, structural and optical properties of $Mg_3Si_2O_5(OH)_4$

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Abstract

We present first principles calculations of structural properties, electronic structure, and optical properties of hexagonal $Mg_3Si_2O_5(OH)_4$ by using the Vienna ab initio simulation package (VASP) within the generalized-gradient approximation (GGA). Using experimentally established lattice parameters as input, full optimization of the geometry of the lattice has been performed. A difference of 3.6% between calculated and experimentally measured volume of the unit cell was found in the present calculations. The total density of states was calculated using the optimized lattice parameters. From that $Mg_3Si_2O_5(OH)_4$ was found to be a wide-band gap material with the calculated band gap exceeding 4 eV. The orbital and site projected density of states show the topmost valence band contains sharp peaks belonging to O atoms, which reveals the ionic nature of the chemical bonds in Lizardite. The lowest conduction band has a strong contribution from the Si 4 *s* hybridized with O 2 *s* electrons. In addition, reflectivity, absorption coefficient, electron–electron loss function, the extinction coefficient, and the refractive index are also studied. We show that the optical properties of Lizardite are isotropic and do not depend on direction. The absorption and reflectivity values are almost zero in the photon energy range 0–4 eV, whereas the Refractive index is ~ 1.58. So, if combined with Si, $Mg_3Si_2H_4O_9$ will possess good antireflection properties while the present of hydrogen will be important to passivate dangling bonds which are at the surface and other bulk defects in Si.

Keywords

- Lizardite;
- Ab-initio calculations;
- Electronic structure;
- Optical properties