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NaAuS chicken-wire-like semiconductor: Electronic structure and optical properties

Abstract

The electronic structure, charge density and optical properties of NaAuS a chicken-wire-like semiconductor was calculated using full potential linear augmented plane wave based on density functional theory. The Ceperley-Alder local density approximation, Perdew Becke Ernzerhof Generalized gradient approximation and Engel Voskov Generalized Gradient Approximation were applied to solve the exchange correlation potential. The investigation of band structures and density of states elucidates that Engle Vasko Generalized Gradient Approximation shows close agreement to the experimental data. The calculated valence charge density shows pure ionic nature of Au–Au bond. It becomes partially covalent when Au is connected with two Na atoms. The linear optical susceptibilities of chicken-wire-like NaAuS semiconductor are calculated so as to obtain further insight into the electronic properties. The uniaxial anisotropy is −0.0005, indicating the strong anisotropy of the dielectric function in the NaAuS a chicken-wire-like semiconductor.

Keywords; Chicken-wire like, Electronic structure, Optical susceptibilities