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First-Principles Calculations of Structural, Elastic, and Electronic Properties of Antiperovskites Ca_3SiO and Ca_3GeO

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ABSTRACT

In this work, we investigated the structural, elastic, and electronic properties of antiperovskites Ca_3SiO and Ca_3GeO, with the full-potential linearized augmented plane wave (FP-LAPW) method. To treat the exchange- correlation potential, we used the local density approximation (LDA) as well as the GGA-PBE and GGA-PBEsol schemes of the generalized gradient approximation (GGA). We employed the Tran-Blaha modified Becke-Johnson generalized gradient approximation (GGA-PBE-mBJ) to perform thecalculations of the electronic properties.

Introduction

Antiperovskites M_3XY (M = metal; X =metalloid; Y = B, C, N, O) attracted a great attention of researchers due to their interesting properties such as superconductivity, giant magnetoresistance, metal-insulator transition, and magnetism[1-5]. Antiperovskites show an inverted occupation of cationic and anionic sites, compared to perovskite materials. Antiperovskites Ca_3SiO and Ca_3GeO crystallize in the cubic $Pm\bar{3}m$ space group (#221). Si or Ge atoms occupy the corners of the unit cell, Olies at the body center, while Ca atoms are located at the face centers of the unit cell.

Theoretical Study

The structural, elastic, and electronic properties of Ca_3SiO, and Ca_3GeO were investigated with FP-LAPW method by using Wien2k package. The cutoff energy, which defines the separation of valence and core states, was chosen as -6 Ry. The Muffin-tin sphere radii were selected as 2.07 a.u. for Ca and O atoms and 2.5 a.u. for Si and Ge atoms. The convergence of the basis set was controlled by a cutoff parameter $R_{mt}*K_{max} = 8$.

Results and Discussion

The lattice parameters obtained with the GGA-PBE approximation are in good agreement with experimental data[6]. By using the GGA-PBE approximation, we investigated the elastic properties of Ca_3SiO and Ca_3GeO. We found that both materials are mechanically stable, elastically anisotropic, and brittle. Calculated Cauchy pressure is negative witch indicates that the directional bonding is predominant in Ca_3SiO and Ca_3GeO. This tendency is confirmed by our calculations of electronic properties which show that Ca_3SiO and Ca_3GeO are narrow-gap semiconductors. Both materials have direct $\Gamma-\Gamma$ gap, equal to 0.15 and 0.22 eV, respectively.

DOI: 10.21467/abstracts.122 ISBN: 978-81-954993-3-5

Conclusion

The investigation of structural, elastic, and electronic properties of Ca_3SiO and Ca_3GeO show that these antiperovskite materials are narrow-gap semiconductors, mechanically stable, elastically anisotropic, and brittle.

Acknowledgments

We thank the DGRSDT (Directorate-General of ScientificResearch and Technological Development - Algeria) for its support.

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ISBN: 978-81-954993-3-5
DOI: 10.21467/abstracts.122
Series: AIJR Abstracts