Contribution ID: **166** Type: **Oral Presentation**

Effect of pressure on structural, mechanical, electronic and optical properties of LiAlS2, NaAlS2 and KAlS2 chalcogenides: A density functional theory study

Tuesday, 4 July 2023 14:40 (20 minutes)

B Phale1, RR Maphanga2, 3 and PS Ntoahae1
1Department of Physics, University of Limpopo, Private Bag x 1106, Sovenga, 0727
2Next Generation Enterprises and Institutions, Council for Scientific and Industrial Research, P.O. Box 395, Pretoria, 0001
3National Institute for Theoretical and Computational Sciences, NITheCS, Gauteng, 2000

Abstract
The structural, mechanical, electronic and optical properties of LiAlS2, NaAlS2 and KAlS2 chalcogenides are investigated by utilizing Perdew-Berke-Ernzerhof functional within generalized gradient approximation under the context of density functional theory as a function of pressure. The mechanical properties are obtained using the Vight-Reuss-Hill approximation. The pressure dependent band structures and density of states are obtained using geometry optimization method. The calculated electronic density of states predict the insulating nature while the band structures exhibit the direct band gaps of 4.21, 3.70 and 3.62 eV for the triclinic LiAlS2, NaAlS2 and KAlS2 respectively, at 0 GPa. The optical properties including the absorption coefficient, refractive index and reflectivity are calculated and analyzed. Furthermore, the spectra of reflectivity curves are high in the ultraviolet regions suggesting they could be used as coating materials to avoid solar heating.

Apply to be considered for a student ; award (Yes / No)?

Yes

Level for award;(Hons, MSc, PhD, N/A)?

MSc

Primary author: Mr PHALE, Boitemogelo (University of Limpopo)

Co-authors: MAPHANGA, Rapela (CSIR); Dr NTOAHAE, Petros (University of limpopo)

Presenter: Mr PHALE, Boitemogelo (University of Limpopo)

Session Classification: Physics of Condensed Matter and Materials Track 2

Track Classification: Track A - Physics of Condensed Matter and Materials