Contribution ID: **94** Type: **Poster Presentation**

First Principles Study of the Properties of K2SbAu Ternary Compound for Energy Harvesting Applications

We are inspired to study the K₂SbAu ternary compound using first-principles methods based on density functional theory (DFT) to advance the optoelectronic technology. This comprehensive study predicts structural, electronic, elastic, mechanical, and optical properties. The lattice parameters of the K₂SbAu ternary compound were in agreement with the experimentally observed values. We observed the structural stability of the K₂SbAu ternary compound using the enthalpy of formation, which was found to be negative, confirming the thermodynamic stability and the possibility of experimental synthesis. The electronic properties suggest narrow indirect band gaps of 0.78 to 1.84 eV using various approximations. The K₂SbAu compound was mechanically stable based on an elastic investigation. Furthermore, we discovered that the compound was ductile, ionic, and anisotropic. The K₂SbAu ternary compound exhibited high optical absorption in the ultraviolet-visible range, suggesting its suitability as a photo absorber in photovoltaic devices. Thus, our findings provide insights for further experimental investigation.

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Session Classification: Poster Session

Track Classification: Track G - Theoretical and Computational Physics