ID 58 – *First principles investigation of structural, elastic, electronic and optical properties of Barium seleno-germate, Ba2GeSe4*

Overview:

Authors modelled the structure and properties of Barium seleno-germate using density functional theory.

They motivated the need for the research and identified the gap in the literature.

The computational details are provided in sufficient detail, such that the computations can be repeated.

The results are structured logically into structural, elastic, electronic and optical properties.

The graphics are clear and annotations are legible.

The conclusions made are consistent with the results that are presented.

There are some minor corrections:

1. Abstract (last line): "…application in multi-junction solar cells."

2. Table 1 caption: "The anble between a…" should be "The angle between…"

3. 3.2 Elastic Properties (line 14): "We therefore…" use of pronouns

4. Table 2: The results show extracted values based on the EOS fitting, but no mention of the errors is made. These results are then compared to experimental values. Is it possible to give an error range on the fitted parameters?

5. The reference format is not applied consistently, please check the use of initials, *et al.* and page numbers.

Recommendation: Accept with minor corrections

Response to corrections

1. The word “cell” was changed to “cells”.

2. “anble” corrected to “angle”.

3. “consider” replaced by “use”

4. In computational materials science it is standard practice not to give error bars for computed results. Information on the computational techniques used are provided instead.

5. The reference format was consistently corrected to the SAIP format.