



Contribution ID: 95

Type: **Poster (sponsored)**

Thermoelectric properties of CdAl₂O₄ spinel

Thermoelectric materials can convert heat into electricity and thermoelectric devices can play an important role in the efficient use of energy. In this study, we investigate the thermoelectric properties of the hard glassy spinel mineral CdAl₂O₄. The potential of a material to be a candidate as the active component of a thermoelectric device is captured in the figure of merit, ZT, which includes information on the lattice and electronic transport properties. Given the difficulties of directly measuring ZT experimentally, we computed its value within density functional theory using linearised Boltzmann transport equations in a relaxation time approximation. We find that CdAl₂O₄ is promising as a high temperature thermoelectric material. For lattice conductivity determination, a supercell of size 2x2x2 consisting of 1476 independent displacements were generated from Phono3py, the calculations were spread on 24 cores adopting MPI program using VASP code.

Presenter Biography

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Session Classification: Poster session

Track Classification: Materials Science