Contribution ID: **108** Type: **Talk**

Density functional theory of thermoelectric properties of graphene

Tuesday, 3 December 2024 11:40 (20 minutes)

Thermoelectricity is the phenomenon direct and thermodynamically reversible conversion of heat to electricity and vice versa. Graphene is one of the carbon-based materials with a low dimensions and mechanically robust, and it tend to have better performance in thermoelectric. Electronic and thermoelectric properties were computed and analysed using density functional theory with a full-potential all-electrons linearised augmented plane waves. The electronic band structure shows a zero band gap with conduction and valence band meeting above the fermi level between the symmetry points H and K. The thermoelectric transport coefficients, Seebeck coefficient, electrical conductivity, thermal conductivity, power factor and figure of merit were calculated using first principle of density of states. Furthermore, a high Seebeck coefficient, electrical conductivity and high power factor were recorded, and these make graphene to be one of the good thermoelectric material and might be applicable for solar cells applications.

Student or Postdoc?

Email address

Co-Authors

CHPC User

Yes

CHPC Research Programme

Workshop Duration

Primary authors: Dr RAMOSHABA, Moshibudi (University of Limpopo); Prof. MOSUANG, Thuto (University of Limpopo)

Presenter: Dr RAMOSHABA, Moshibudi (University of Limpopo)

Session Classification: HPC Applications

Track Classification: Materials Science