Contribution ID: **52** Type: **Poster Presentation**

Lattice thermal conductivity of bulk PtSe₂ and PtTe₂

Thursday, 28 June 2018 15:00 (2 hours)

Thermoelectric devices can play a role in efficiently using available energy by converting heat produced by a wide range of devices into electricity. Low lattice thermal conductivity is a requirement for efficient thermoelectric devices and layered materials offer potential in reducing the lattice thermal conductivity perpendicular to the layers. We present
density functional theory calculations of the structural and thermal properties of layered platinum dichalcogenides PtSe₂ and PtTe₂ compounds in the CdI₂ structure, space group P3m1. Phonon and elastic constants calculations confirm that the compounds are dynamically and mechanically stable. Lattice thermal conductivities were calculated within the single-mode relaxation-time approximation of the linearised phonon Boltzmann equation. We found that at the room temperature, the in-plane lattice thermal conductivities for PtSe₂ and PtTe₂ are 9.33 and 6.54 Wm⁻¹ K⁻¹ , while perpendicular to the plane they are 2.06 and 1.8 Wm⁻¹ K⁻¹ , respectively. The out-of-plane thermal conductivities confirm that further investigation of PtSe₂ and PtTe₂ as thermoelectric materials is necessary.

Please confirm that you
have carefully read the
abstract submission instructions
under the menu item
”Call for Abstracts”
(Yes / No)

yes

Consideration for
student awards
Choose one option
from those below.
N/A
Hons
MSc
PhD

PhD

Supervisor details
If not a student, type N/A.
Student abstract submision
requires supervisor permission:
please give their name,
institution and email address.

Daniel P. Joubert
University of the Witwatersrand, Johannesburg, Wits 2050,
daniel.joubert2@wits.ac.za

Primary author: Mr MOHAMMED, Hamza (University of Witwatersrand)

Co-authors: Prof. JOUBERT, Daniel (university of the Witwatersrand); Dr NGUIMDO, Dongho (African Institute for Mathematical Sciences-Cameroon)

Presenter: Mr MOHAMMED, Hamza (University of Witwatersrand)

Session Classification: Poster Session 2

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