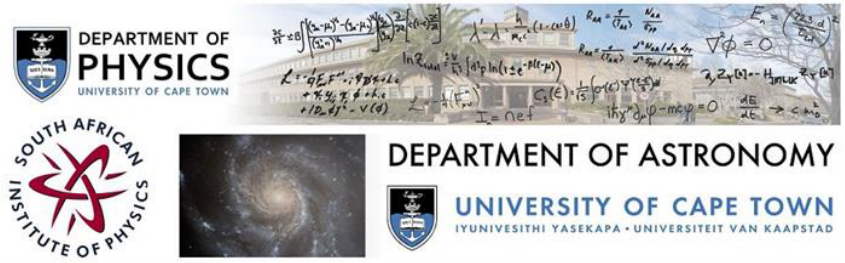

Contribution ID: **457** Type: **Oral Presentation**

Lattice thermal conductivity properties of three binary type- I Sn clathrates from Density Functional Theory

Tuesday, 5 July 2016 14:00 (20 minutes)

Abstract content
   (Max 300 words)
Formatting &
Special chars

A low thermal conductivity material is a good choice for a thermoelement provided the power factor is not affected adversely. In this study, the suppression of thermal conductivity, using the high temperature phase in the three binary type-I Sn clathrates, Cs8Sn44, K8Sn44 and Rb8Sn44 was studied using Density Functional Theory in the Local Density
approximation. Analysis of the projected density of state suggests a decoupled oscillations of the guest atoms which is believed to scatter the acoustic phonons and hence reduce the lattice thermal conductivity [1]. Using ab initio molecular dynamics phonon calculations, an indication of any anharmonicity was investigated. Our result is confirmed by a detailed analysis of the lattice vibrations and the role the guest atoms play in reducing the lattice thermal conductivity from similar studies using Raman spectroscopy and inelastic neutron scattering [2].

[1] Voneshen, D. J., Refson, K., Borissenko, E., Krisch, M., Bosak, A., Piovano, A., ... & Roger, M. (2013). Suppression of thermal conductivity by rattling modes in thermoelectric sodium cobaltate. Nature materials, 12(11), 1028-1032.
2] Christensen, Mogens, Fanni Juranyi, and Bo B. Iversen. "The rattler effect in thermoelectric clathrates studied by inelastic neutron scattering." Physica B: Condensed Matter 385 (2006): 505-507.

Apply to be
 considered for a student
   award (Yes / No)?

Yes

Level for award
 (Hons, MSc,
   PhD, N/A)?

PhD

Main supervisor (name and email)
and his / her institution

Prof. Daniel P Joubert [daniel.joubert2@wits.ac.za]
University Of Witwatersrand, Johannesburg

Would you like to
 submit a short paper
 for the Conference
 Proceedings (Yes / No)?

Yes

Please indicate whether
this abstract may be
published online
(Yes / No)

Yes

Primary author: Mr EGBELE, Peter (University of Witwatersrand, Johannesburg)

Co-author: Prof. JOUBERT, Daniel (University of Witwatersrand, Johannesburg)

Presenter: Mr EGBELE, Peter (University of Witwatersrand, Johannesburg)

Session Classification: Theoretical and Computational Physics (1)

Track Classification: Track G - Theoretical and Computational Physics