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First-principles investigation of lattice thermal conductivity and stuctural stability of CH₃NH₃PbI₃

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The stuctural stability, elastic constants, vibrational properties and lattice thermal conductivity of the orthorhombic CH₃NH₃PbI₃ have been investigated using first-principles calculations. These calculations were based on density functional theory and were performed using a generalized gradient approximation parametrized by Perdew, Burke and Ernzerhof (PBE and PBEsol). The relaxed system is dynamicaly satble, while the equilibrium elastic constants satisfy all the mechanical stability criteria for an orthorhombic structure, showing stability against small distortions. The lattice thermal conductivity was calculated with the single-mode relaxation-time approximation and a full solution of the linearized phonon Boltzmann equation from first-principles anharmonic lattice dynamics calculations. We found that the lattice thermal conductivity of CH₃NH₃PbI₃ is non-isotropic, with values of 0.134, 0.083, and 0.43 W m⁻¹ K⁻¹ in the directions x, y and z, respectively.

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

Daniel Joubert
daniel.joubert2@wits.ac.za
The National Institute for Theoretical Physics, School of Physics and Mandelstam Institute for Theoretical Physics,
University of the Witwatersrand, Johannesburg, Wits 2050, South Africa.

Would you like to
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 for the Conference
 Proceedings (Yes / No)?

yes

Primary author: Mr ABDALLAH, Ibrahim (School of Physics and Mandelstam Institute for Theoretical Physics, University of the Witwatersrand)

Co-authors: Prof. JOUBERT, Daniel (School of Physics and Mandelstam Institute for Theoretical Physics, University of the Witwatersrand, Johannesburg, Wits 2050, South Africa.); Dr SULEIMAN, Mahammed (Department of Basic Sciences, Imam Abdulrahman Bin Faisal University, Dammam, KSA.)

Presenter: Mr ABDALLAH, Ibrahim (School of Physics and Mandelstam Institute for Theoretical Physics, University of the Witwatersrand)

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