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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 Wm¹ 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 <

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Session Classification: Poster Session 2

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