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Lattice thermal conductivity of bulk WSe2

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Thermoelectric devices can convert heat into an electric current and have immense potential for efficient use available energy. This includes converting heat energy from internal combustion engines, conventional power plants and solar cells into usable energy. Research into finding efficient thermoelectric materials has intensified over the past decade. One of the desired features of efficient thermoelectric materials is a low lattice thermal conductivity. In other words, the thermal energy transported by the motion of the atoms in a thermoelectric materials should be small. Recent research suggests that some layered materials may be materials with this property. In this study we used first-principle calculations to investigate the structural, electronic, and vibrational properties of bulk WSe2 , a layered material. The lattice thermal conductivity was calculated by using a single-mode relaxation-time approximation in the linearized phonon Boltzmann equation from first-principles an-harmonic lattice dynamics calculations. We find that the lattice thermal conductivity of WSe2 is non-isotropic, with a value of 63.78 Wm−1K−1 in the direction of the plane and 2.39 W m −1 K −1 perpendicular to the plane at room temperature. The thermal conductivity perpendicular to the plane is close to experimental value at room temperature, and is in a range which makes this an interesting material as a potential active component in a thermoelectric device.

Apply to be
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yes

Level for award
 (Hons, MSc,
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PhD

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

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Would you like to
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yes

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