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Thermoelectric properties of CH₃NH₃PbI₃ using density functional theory and Boltzmann transport calculations

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The thermoelectric properties of organic-inorganic halide perovskite CH₃NH₃PbI₃ were studied by solving the semiclassical Boltzmann transport equations on top of density functional theory calculations by using maximally-localised Wannier functions (MLWFs). Electronic transport properties were evaluated within the constant relaxation time approximation at four different temperatures 300 K, 500 K, 700 K, and 900 K. The electrical conductivity (σ) was found to be almost constant in the entire temperature range, while the Seebeck coefficient (S) was found to decrease with increasing temperature and the electronic thermal conductivity (κ) was found to increase with increasing temperature. Theoretical results for the power factor (S² σ) and the figure of merit (ZT) are analysed. The highest predicted average figure of merit is 0.85 at 900 K.

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

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

yes

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