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First principle studies on lattice thermal conductivity and thermoelectric properties of LiYSe<sub>2<sub>

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Thermoelectric materials can convert heat into electricity and thermoelectric devices can play an important role in the efficient use of energy. In this study, we investigate structural, dynamical and mechanical stability of LiYSe<sub>2<sub> alongside its lattice thermal conductivity and thermoelectric properties for the first time. The ability of a material to be a applied as the active component in the design of a thermoelectric device is based on the magnitude of its figure of merit, ZT, which includes information on the lattice and electronic transport properties. Given the difficulties of directly measuring ZT experimentally, we computed its value within density functional theory using linearized Boltzmann transport equations in a relaxation time approximation.

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

Yes

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

PhD

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