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Ab initio thermal transport in strongly anharmonic materials OLLE HELLMAN, California Institute of Technology — We present recent advances regarding the temperature dependent effective potential method (TDEP) and its application to thermoelectric materials. All orders of non-harmonic effects are implicitly included when calculating phonon dispersions, lattice thermal transport and finite temperature phase stability. Recent additions deal with thermal transport in disordered systems, complex crystal structures and numerical efficiency for high-throughput applications.

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