



Award #: 1931436

CSSI Element: Enabling Accurate Thermal Transport Calculations in LAMMPS

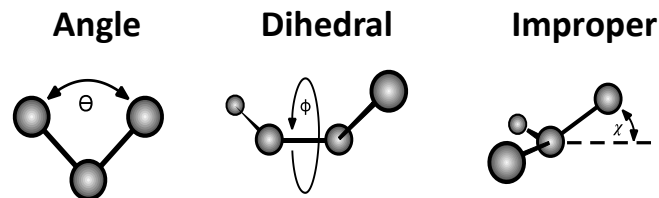
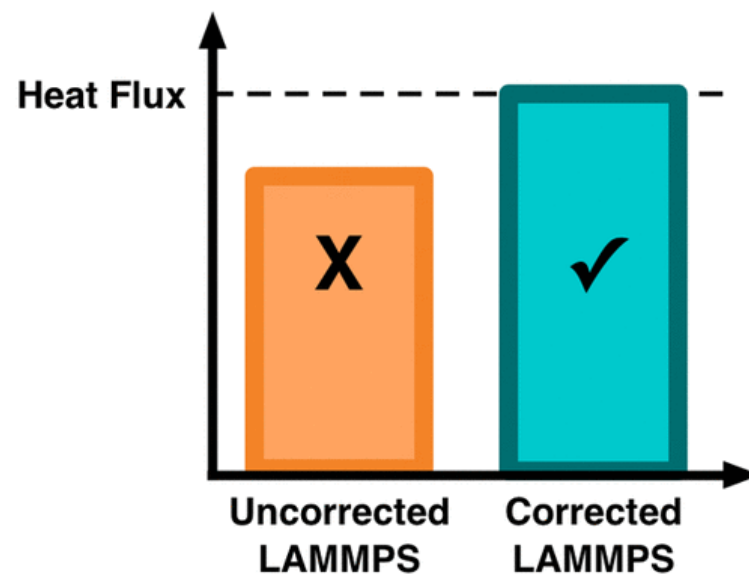
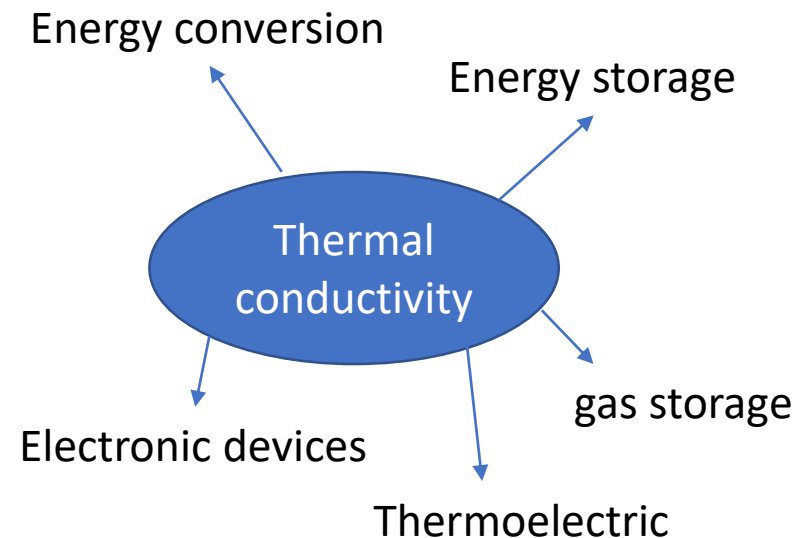
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Thermal conductivity is important
in many energy applications

No MD code can calculate heat flux correctly

Project Objectives



- Implement the corrected heat flux computation for all supported many-body potentials in LAMMPS
- Identify the types of molecular systems most affected by the changed heat flux computations
- Apply and refine the methodology to predict thermal conductivity for several novel nanomaterial