CSSI Element: Enabling Accurate Thermal Transport Calculations in LAMMPS

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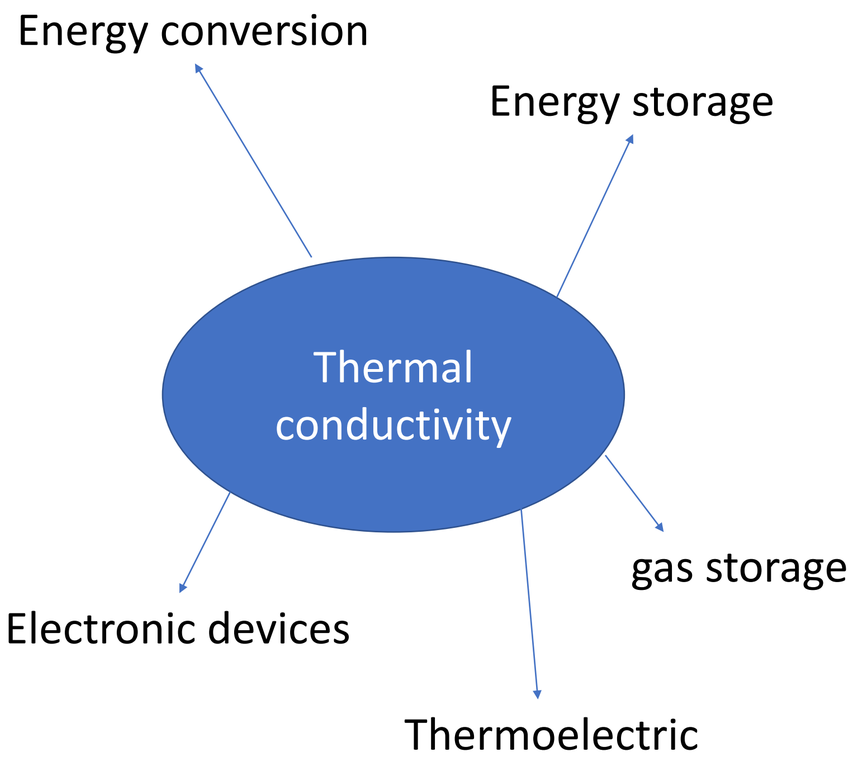
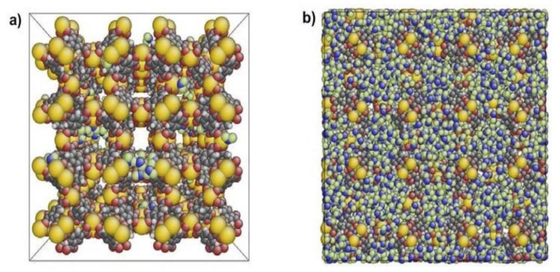
Motivation

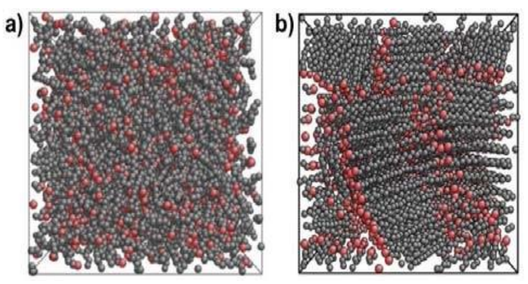
✓ Thermal conductivity is important in many energy applications



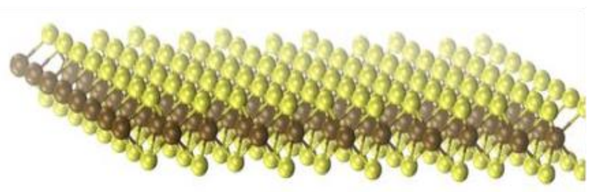
Rapid gas adsorption in porous materials



Phase change materials for energy storage

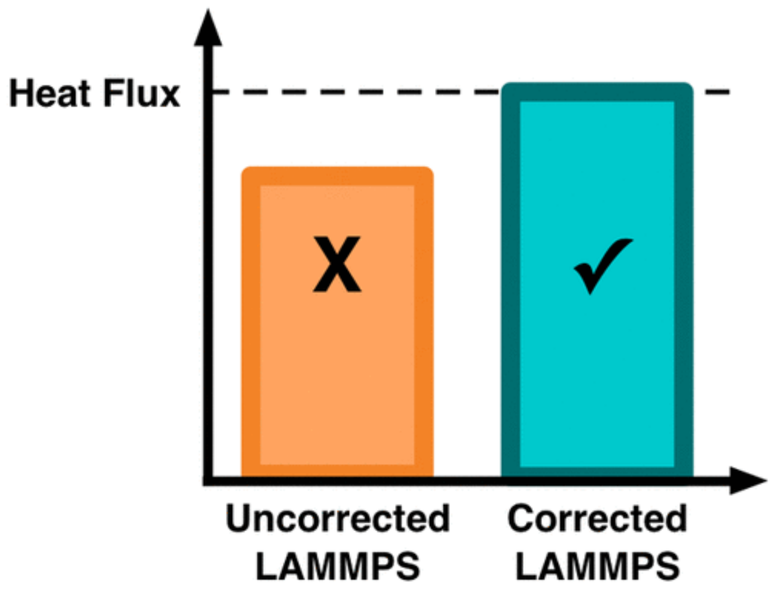


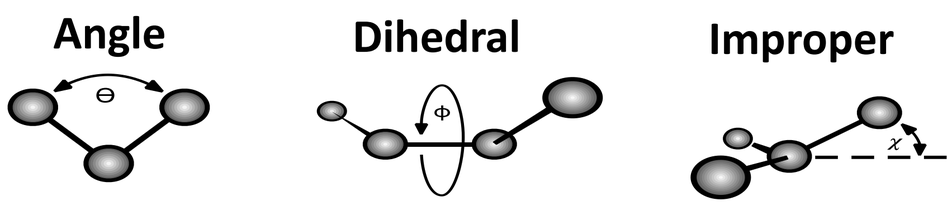
Thermoelectric materials



Wherever measuring an accurate **thermal conductivity** via **Green-Kubo** is important…

✓ No MD code can calculate heat flux correctly





LAMMPS heat flux definition **NOT OK for multi-body terms!**

$$(JV)_{n-body,uncorrected} = \sum_{i}^{atoms} \boldsymbol{v_i} \cdot \left[\sum_{\{s_1, s_2 \ldots i \ldots s_n\}}^{n-bodies} \frac{1}{n} \left[\sum_{j=1}^{n} \boldsymbol{r_{s_j}} \otimes \boldsymbol{F_{s_j}} \right] \right]$$

Corrected definition **OK!**

$$(JV)_{n-body,corrected} = \sum_{\{s_1, s_2 \ldots s_n\}}^{n-bodies} \left[\frac{1}{n} \sum_{j=1}^{n-1} \sum_{k>j}^{n} \left(\boldsymbol{F_{s_j}} \cdot \boldsymbol{v_{s_j}} - \boldsymbol{F_{s_k}} \cdot \boldsymbol{v_{s_k}} \right) \boldsymbol{r_{s_j s_k}} \right]$$

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

Broader Impacts

- The proposed research will enable large-scale computational screening of materials to accurately predict their thermal properties-- Materials Genome Initiative (MGI)
- responds directly to NSCI strategic objective 4 in the NSCI 2016 strategic plan:
  - ✓ innovative, scalable, reusable software component that supports the mission needs of the NSF and CBET
  - ✓ it supports training for the broad LAMMPS user community as well as general workforce development via training to undergraduates
  - ✓ it ensures the new software capacities proposed are widely available via the open-source LAMMPS package