Large-Scale, GPU-Enhanced DFTB Approaches for Probing Multi-Component Alloys
Anshuman Kumar1, Sarah I. Allec1, Bryan M. Wong1,2
Department of Materials Science & Engineering, University of California, Riverside
Department of Chemical & Environmental Engineering, University of California, Riverside

Introduction

- Achieving maximum theoretical performance of structural alloys requires searching a large compositional phase space
- Computational screening will accelerate and guide design & synthesis of multi-component alloys at elevated temperatures for fossil energy power plant technologies
- Need to balance accuracy and efficiency
- → GPU-enhanced Density Functional Tight-Binding (DFTB)

Theoretical Methods

- Density Functional Tight-Binding (DFTB)1
  - Minimal atomic orbital basis
  - Treat valence electrons in field of nuclei & core electrons
  - Taylor series expansion of Kohn-Sham total energy:
    \[ E[p] = E_0[p_\text{0}] + E_1[p_\text{0}, \delta p] + E_2[p_\text{0}, (\delta p)^2] + \cdots \]
  - Truncate at 2nd order term → DFTB2
    \[ E_{\text{DFTB}} = E_{\text{rep}} + \sum_{\text{non-SCC } H} \sum_{\text{parametrized}} \Delta q_{\alpha \beta} \Delta q_{\gamma \delta} F_{\alpha \beta} \]
- \( E_{\text{rep}} \) lumps together difficult many-body effects (e.g., exchange-correlation)
- \( H_0 \) and overlap matrix elements parametrized beforehand from DFT calculations

GPU Enhancements

- Used modified GPU-enhanced version of DFTB+
  - Parallelized diagonalization of \( \hat{H} \) with NVIDIA K80 GPUs

Results

- DFTB parametrization2 of iron (Fe)
  1. Tabulate Hamiltonian and overlap matrix elements as function of distance.
  2. Calculate repulsive potential, \( E_{\text{rep}} = E_{\text{DFT}} - E_{\text{DFTB}} \), for several reference systems.

References


Contact
Name: Prof. Bryan M. Wong
Email: bryan.wong@ucr.edu
Website: http://www.bmwong-group.com

Acknowledgements
This work was supported by the National Energy Technology Laboratory (NETL) of the U.S. Department of Energy under Award No. DE-FE0030582.