Large-Scale, GPU-Enhanced DFTB Approaches for Probing Multi-Component Alloys

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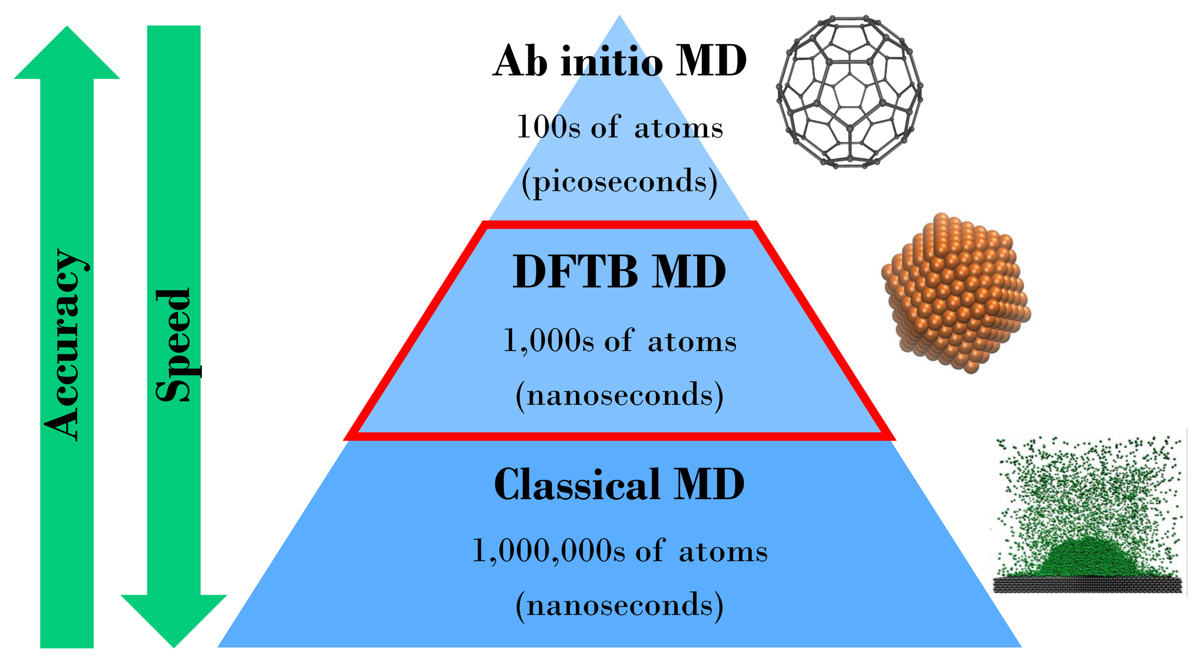
Introduction

- 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*:

$$E[\rho] = E^0[\rho_0] + E^1[\rho_0, \delta\rho] + E^2[\rho_0, (\delta\rho)^2] + \cdots$$

  - Truncate at 2nd order term → DFTB2

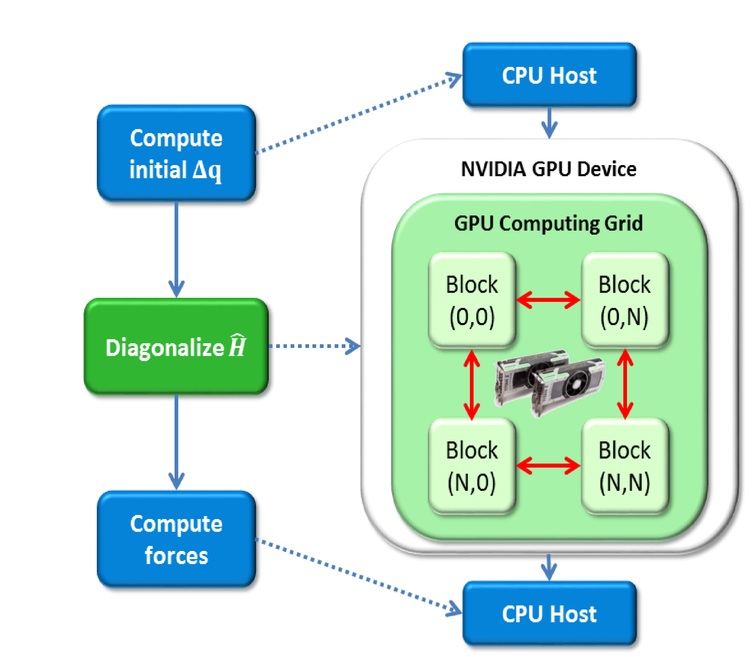
$$E_{\mathrm{DFTB2}} = E_{rep} + \sum_i^{occ} \langle \phi_i | H_0 | \phi_i \rangle + \frac{1}{2} \sum_{\alpha,\beta}^{N} \Delta q_\alpha \Delta q_\beta \gamma_{\alpha\beta}$$

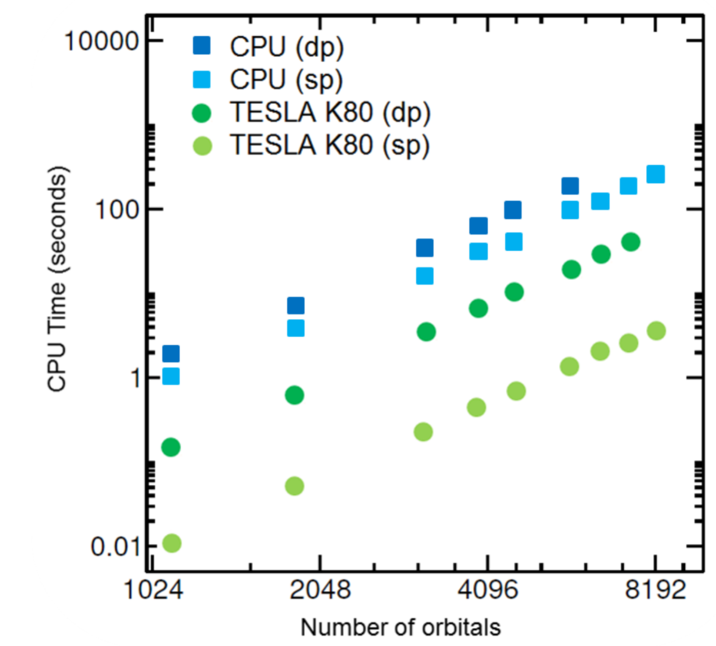
Short-range repulsion (E_{rep}) · non-SCC H (parametrized) · Long-range electrostatic interactions

- E_{rep} lumps together difficult many-body effects (e.g., exchange-correlation)
- H_0 and overlap *matrix elements parametrized beforehand* from DFT calculations

GPU Enhancements

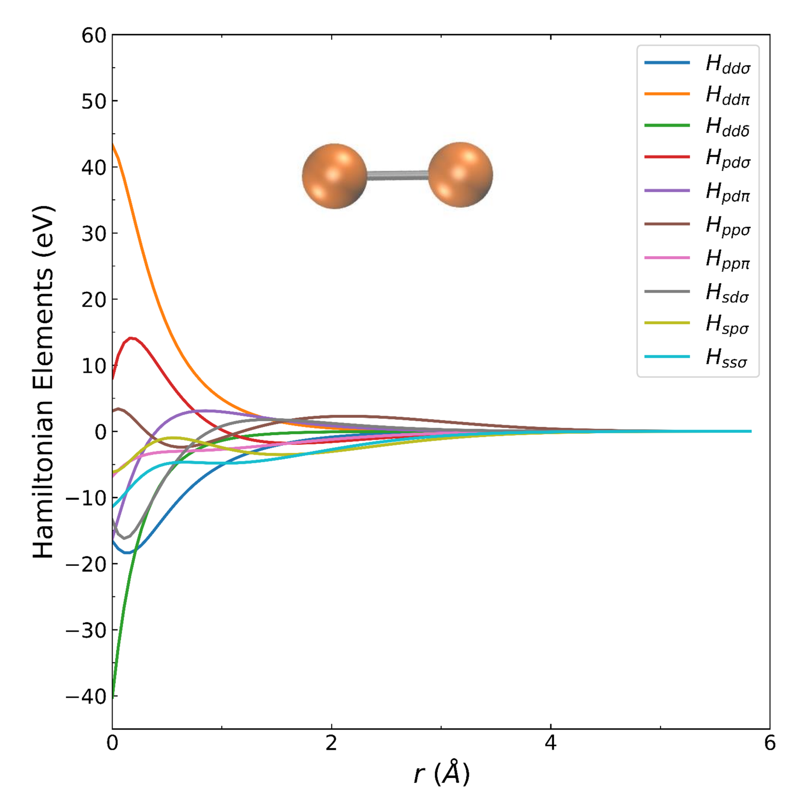
- Used modified GPU-enhanced version of DFTB+
  - Parallelized diagonalization of $\hat{H}$ with NVIDIA K80 GPUs

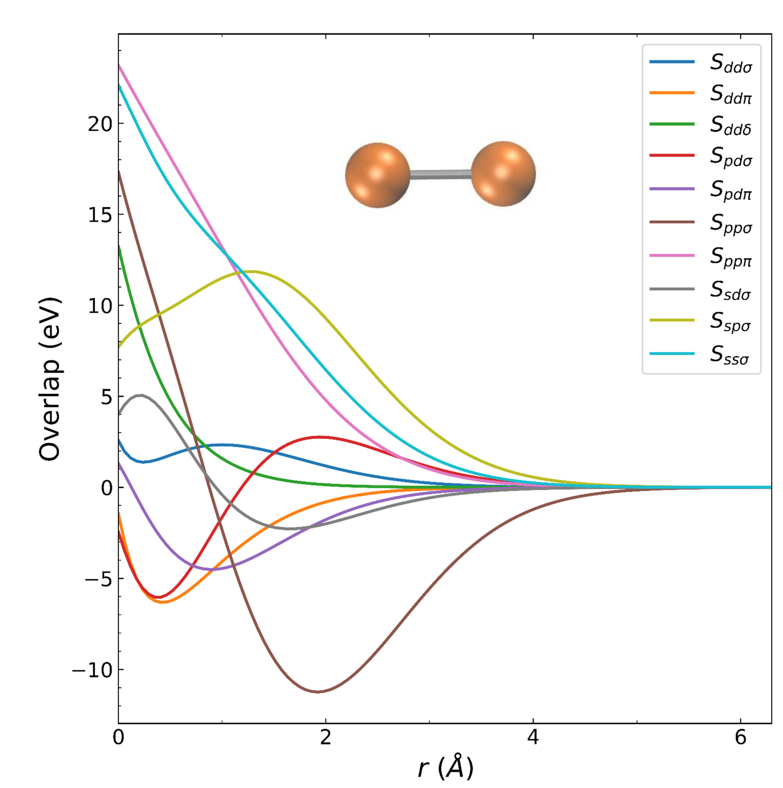




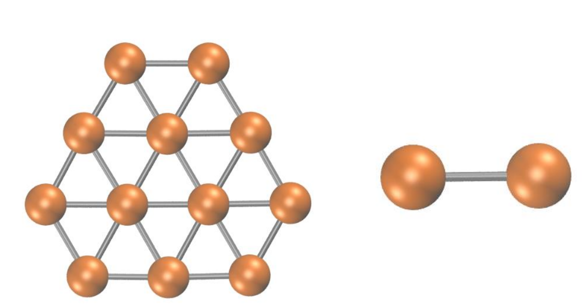
Results

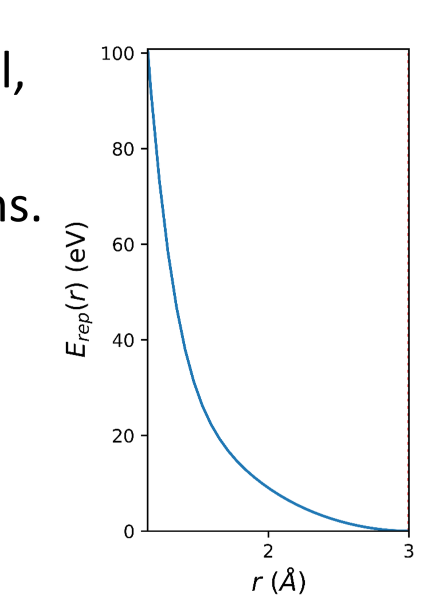
- DFTB parametrization[2] of iron (Fe)
  1. Tabulate Hamiltonian and overlap matrix elements as function of distance.

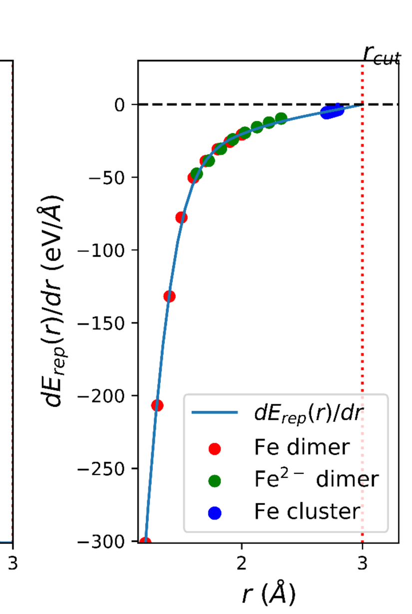




  2. Calculate repulsive potential, $E_{rep} = E_{DFT} - E_{DFTB}$, for several reference systems.

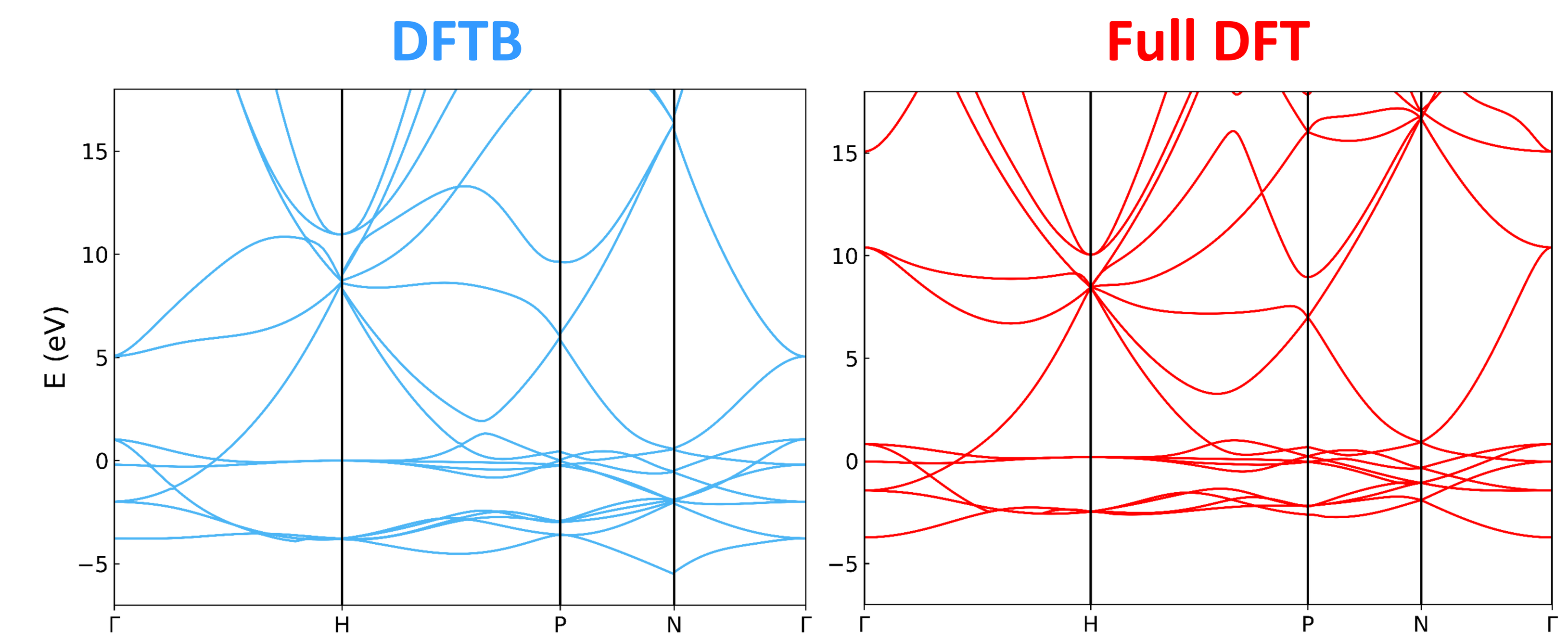


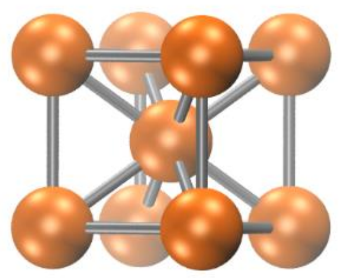




Results

- Band structure of BCC iron using DFTB with our parametrization vs. full DFT





$$\sum_\alpha H_{\alpha'\alpha}(\boldsymbol{k}) c_\alpha(\boldsymbol{k}) = E c_{\alpha'}(\boldsymbol{k})$$

$$H_{\mu\nu}(\boldsymbol{r}) = \langle \phi_\mu(\boldsymbol{r}) | H^o | \phi_\nu(\boldsymbol{r} - \boldsymbol{r_o}) \rangle \ , S_{\mu\nu}(\boldsymbol{r}) = \langle \phi_\mu(\boldsymbol{r}) | \phi_\nu(\boldsymbol{r} - \boldsymbol{r_o}) \rangle$$

$$H^o = -\frac{1}{2}\nabla^2 + v_{eff}[\rho^a(\boldsymbol{r})] + v_{eff}[\rho^b(\boldsymbol{r} - \boldsymbol{r_o})]$$

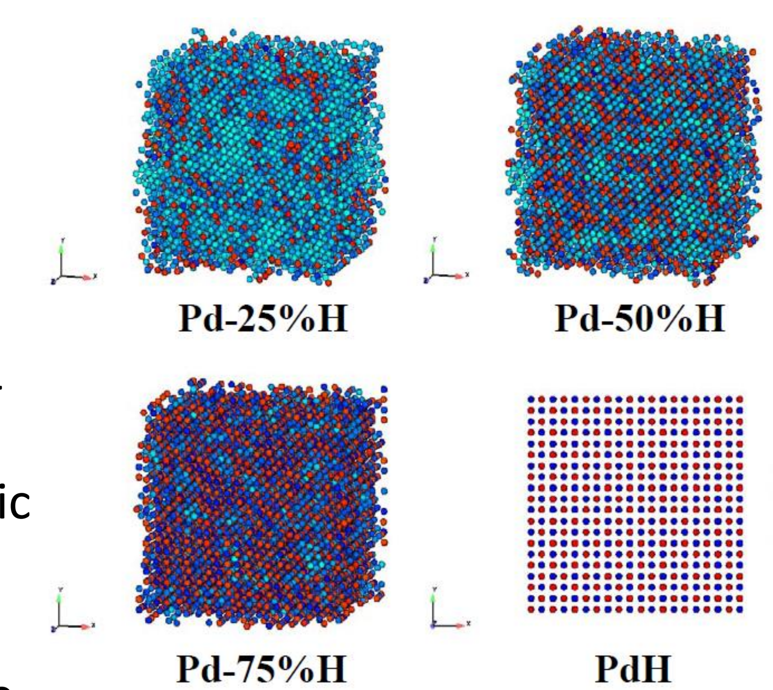
Conclusions & Future Work

Conclusions

- Parallelized diagonalization of $\hat{H}$
  - 1.5x faster evaluation
- Parametrized iron (Fe)

Future work

- Create parameter sets for other relevant elements (e.g., Ni, Cr) & interactions (e.g., Fe-Ni, Fe-Cr)
- Optimize parameters with genetic algorithms
- Predict structural properties for alloys as function of temperature



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2. Koskinen, P.; Makinen V. Density-functional tight-binding for beginners. *Comput. Mater. Sci.* **2009**, *47*, 237-253.