EAM vs. DFT – fcc and hcp phases
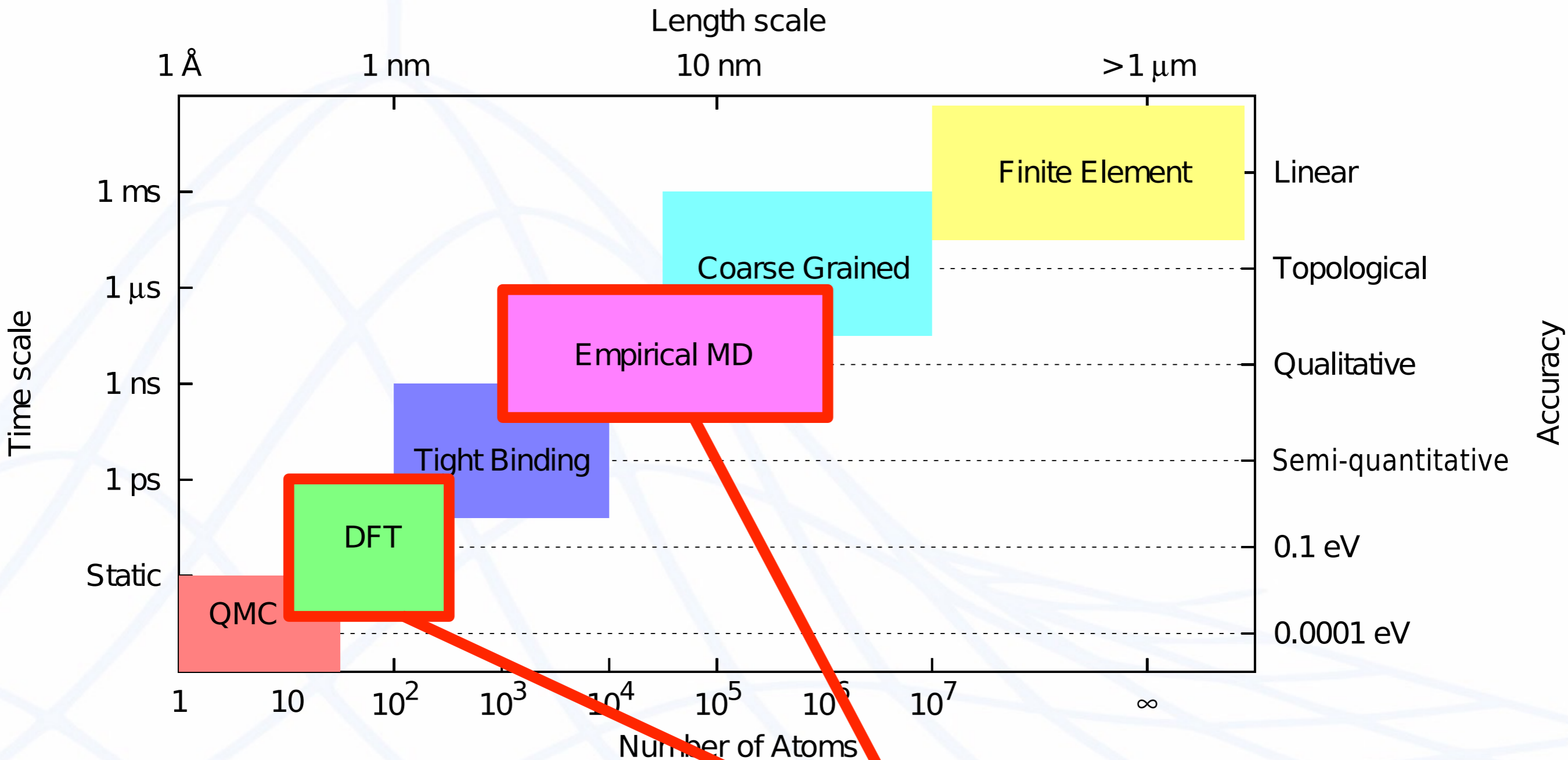

0K stacking fault energy profile
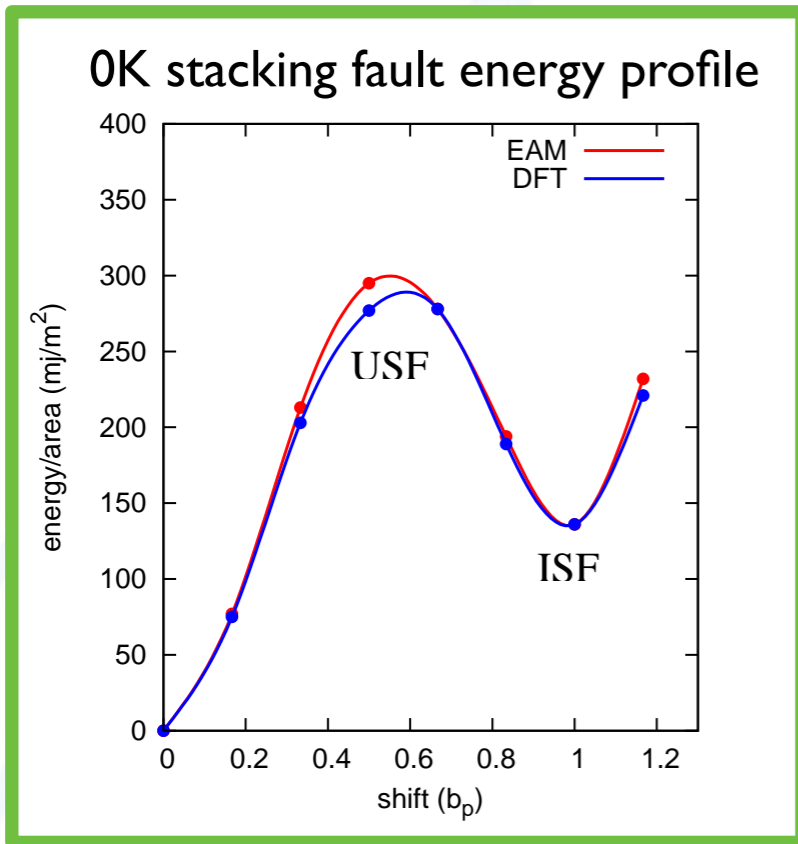
Included in fitting set

Energy vs. strain plots for Ni

fcc

hcp

Pair interaction

Electron density term

$$E_{tot} = \frac{1}{2}\sum_{i,j=1}^{\mathcal{N}} \phi_{ij}(r_{i,j}) + \sum_{i=1}^{\mathcal{N}} \mathcal{F}_i(\bar{\rho}_i)$$

EAM Ni-Ni energy contributions
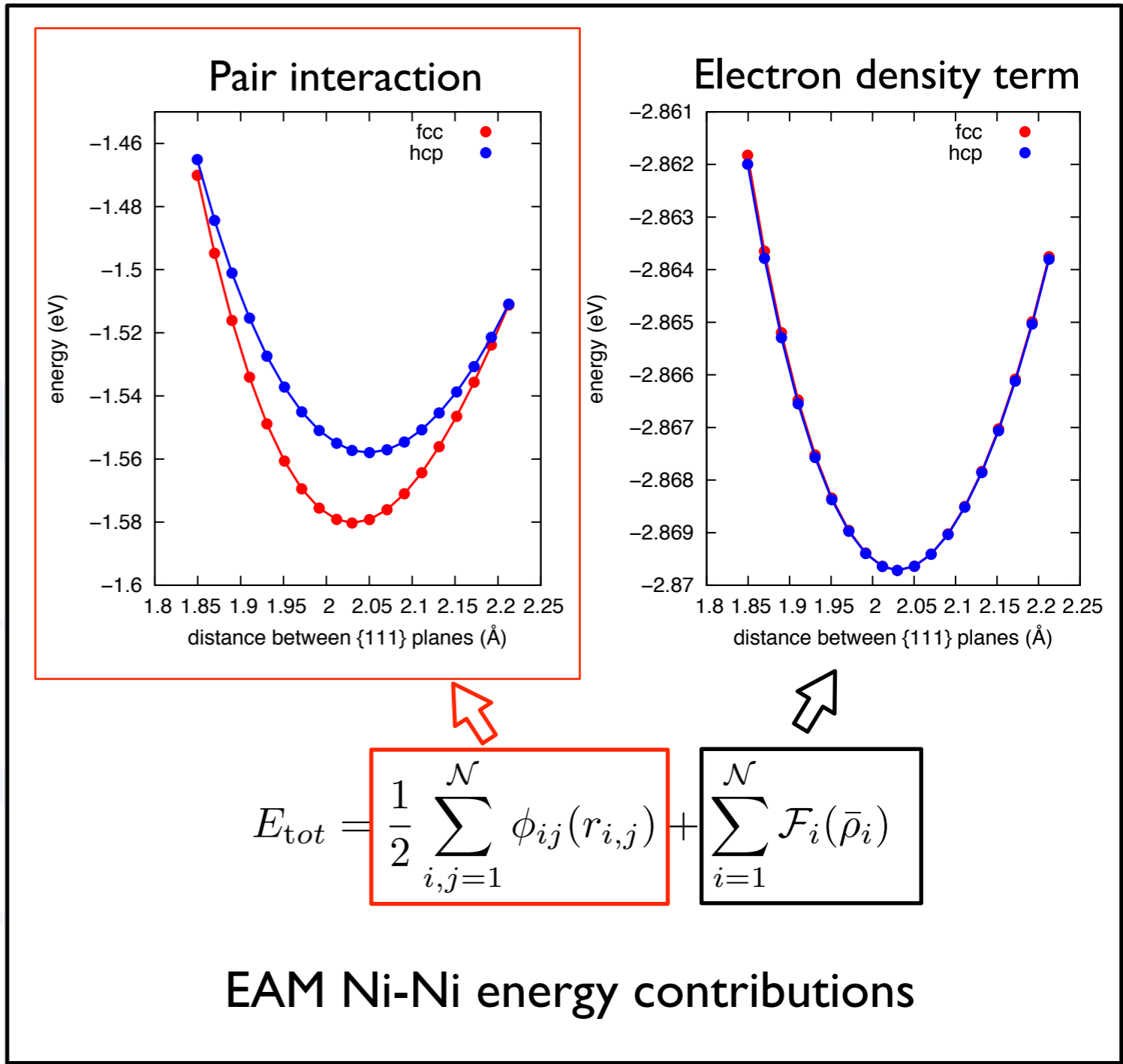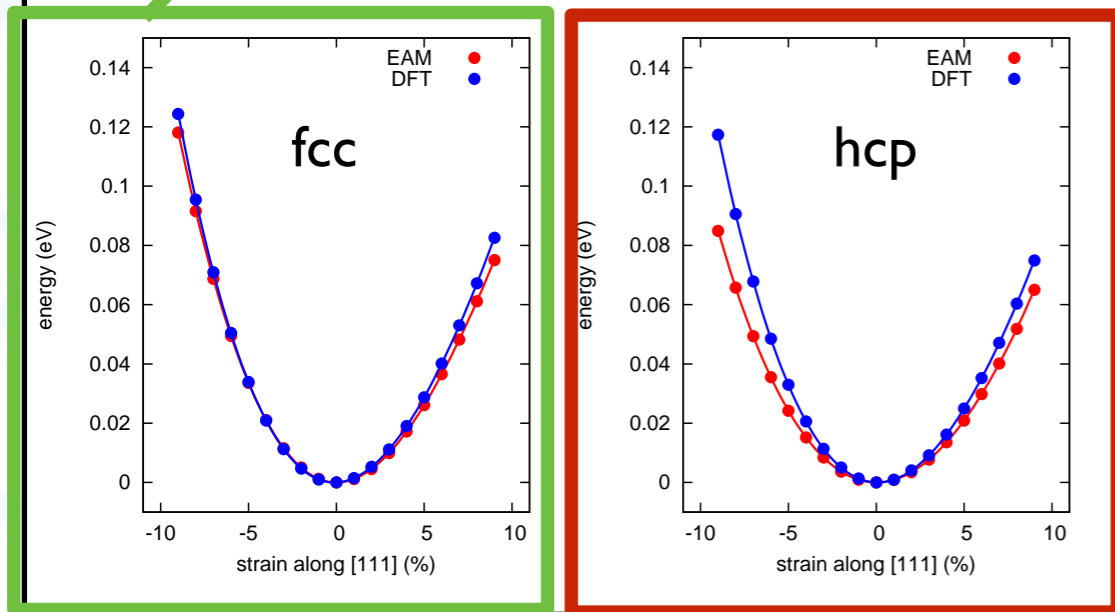
hcp elastic properties not included in fitting!

Concurrent Multiscale Materials Modelling