Multi-Scale Modeling of Phase-Change Memory (PCM) Materials

What we are doing with DFT:

- ✓ Probing energy hypersurface (different structural configurations) of PCM GeTe, Sb_2Te_3, $Ge_2Sb_2Te_5$.
- ✓ Fitting classical interatomic potentials to these hypersurfaces.
- ✓ Using classical potentials to run large-scale MD simulations.
- ✓ Exploring wavelet DFT as a method to drive MD simulations of PCM materials.