

**Supplementary information for “Automated crystal characterization with a fast
Neighborhood Graph Analysis method”**

Wesley F. Reinhart and Athanassios Z. Panagiotopoulos

*Department of Chemical and Biological Engineering, Princeton University,
Princeton, NJ 08544, USA*

(Dated: 9 May 2018)

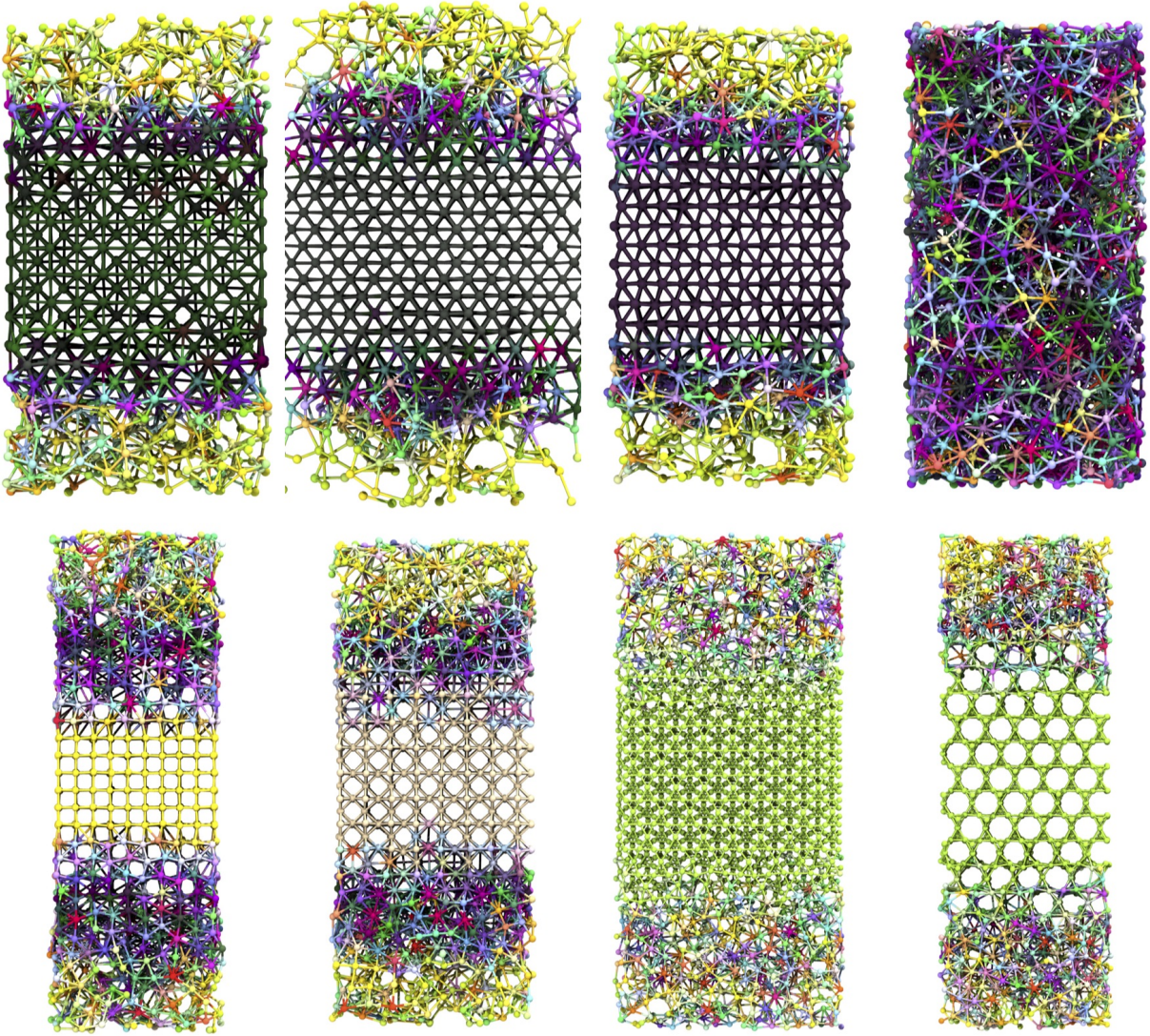


FIG. S1: Snapshots of thermalized crystal lattices colored according to the diffusion map of Fig. 3, built from first-degree neighborhood graphs. Top row: BCC, FCC, HCP, liquid. Bottom row: SC, perovskite, CT, HT.

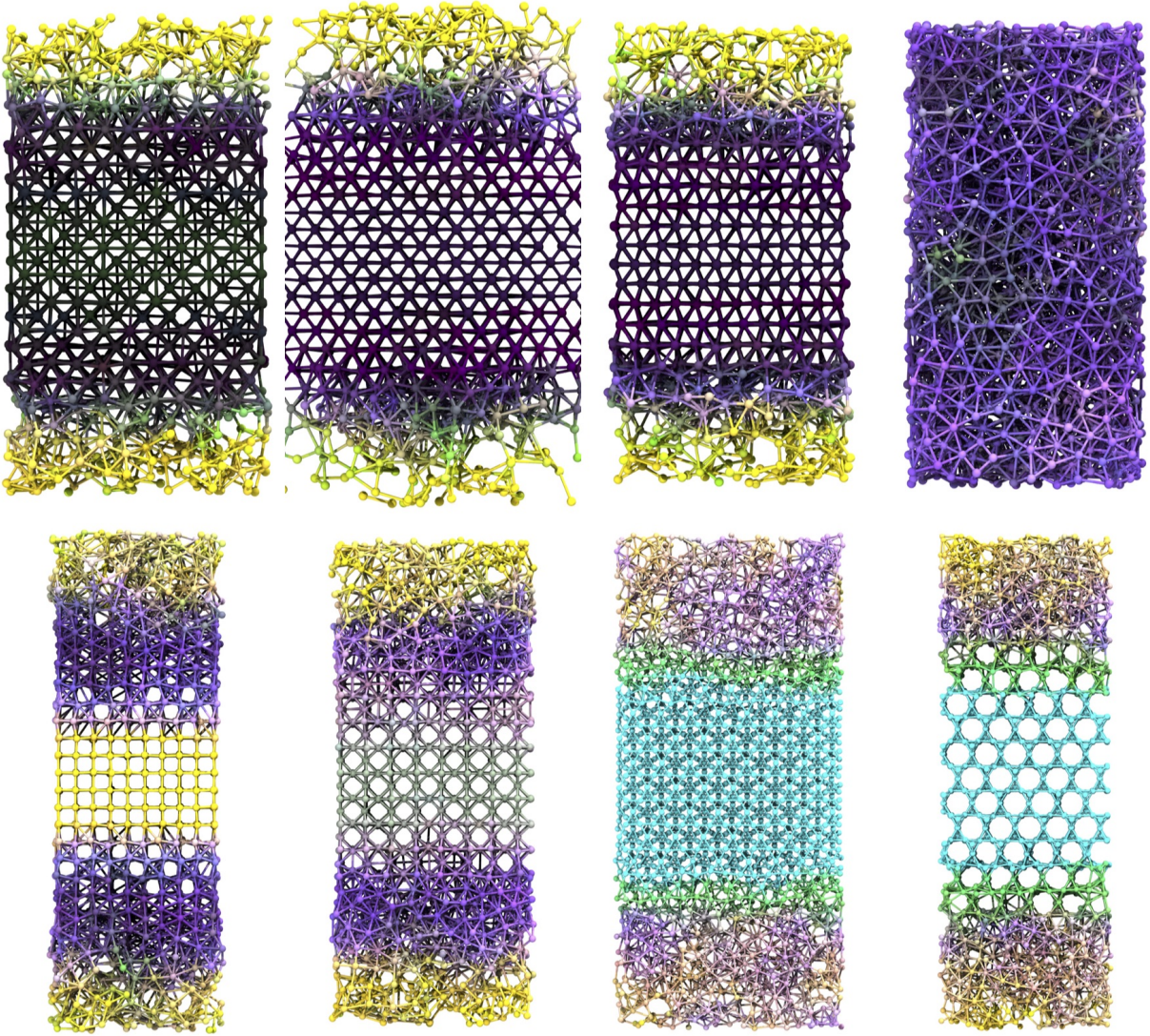


FIG. S2: Snapshots of thermalized crystal lattices colored according to the diffusion map of Fig. 4, built from third-degree neighborhood graphs. Top row: BCC, FCC, HCP, liquid. Bottom row: SC, perovskite, CT, HT.