

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

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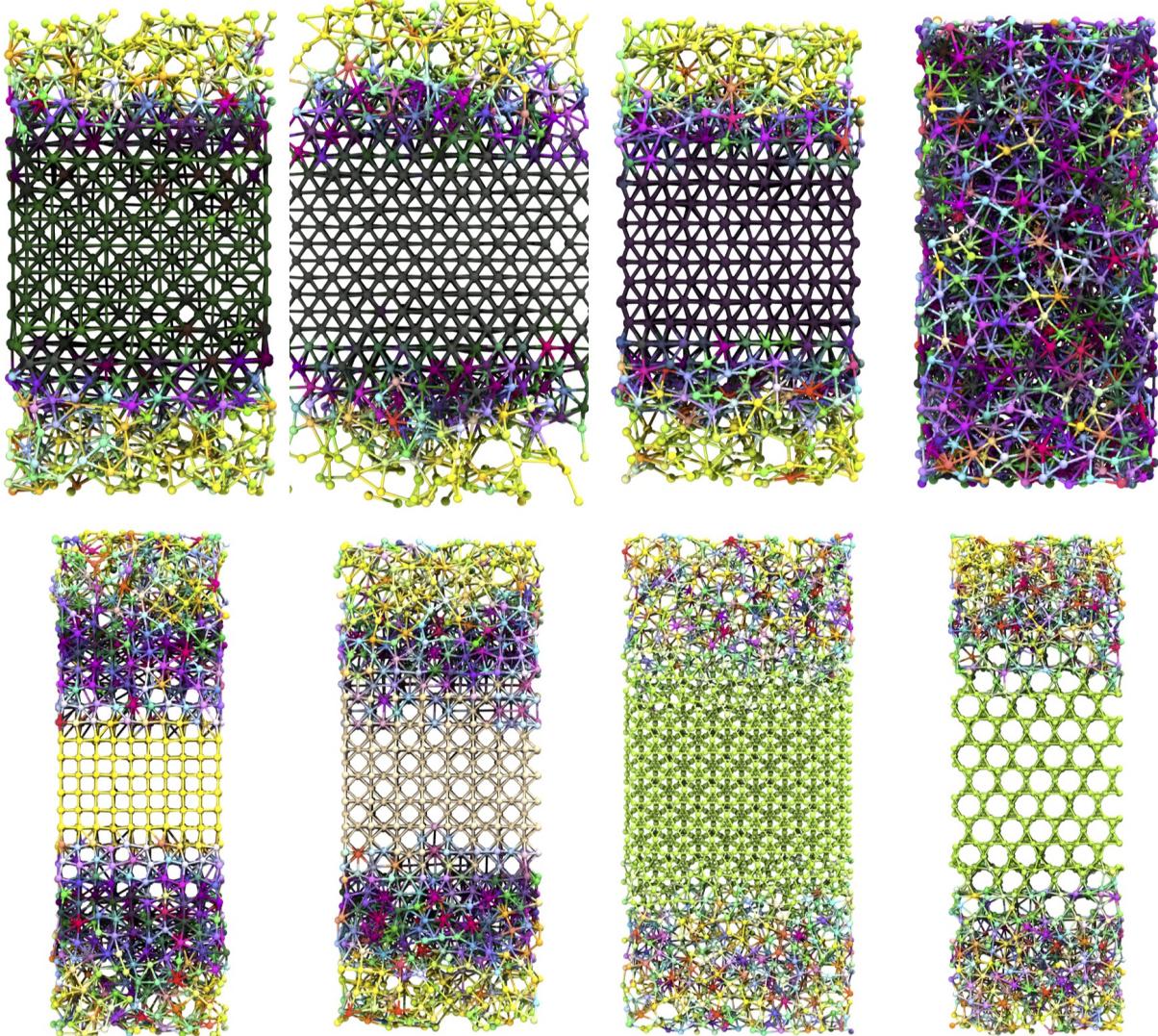


FIG. S1: Snapshots of thermalized crystal lattices colored according to the diffusion map of Fig. 3, built from first-degree neighborhood graphs. Top row: BCC, FCC, HCP, liquid. Bottom row: SC, perovskite, CT, HT.

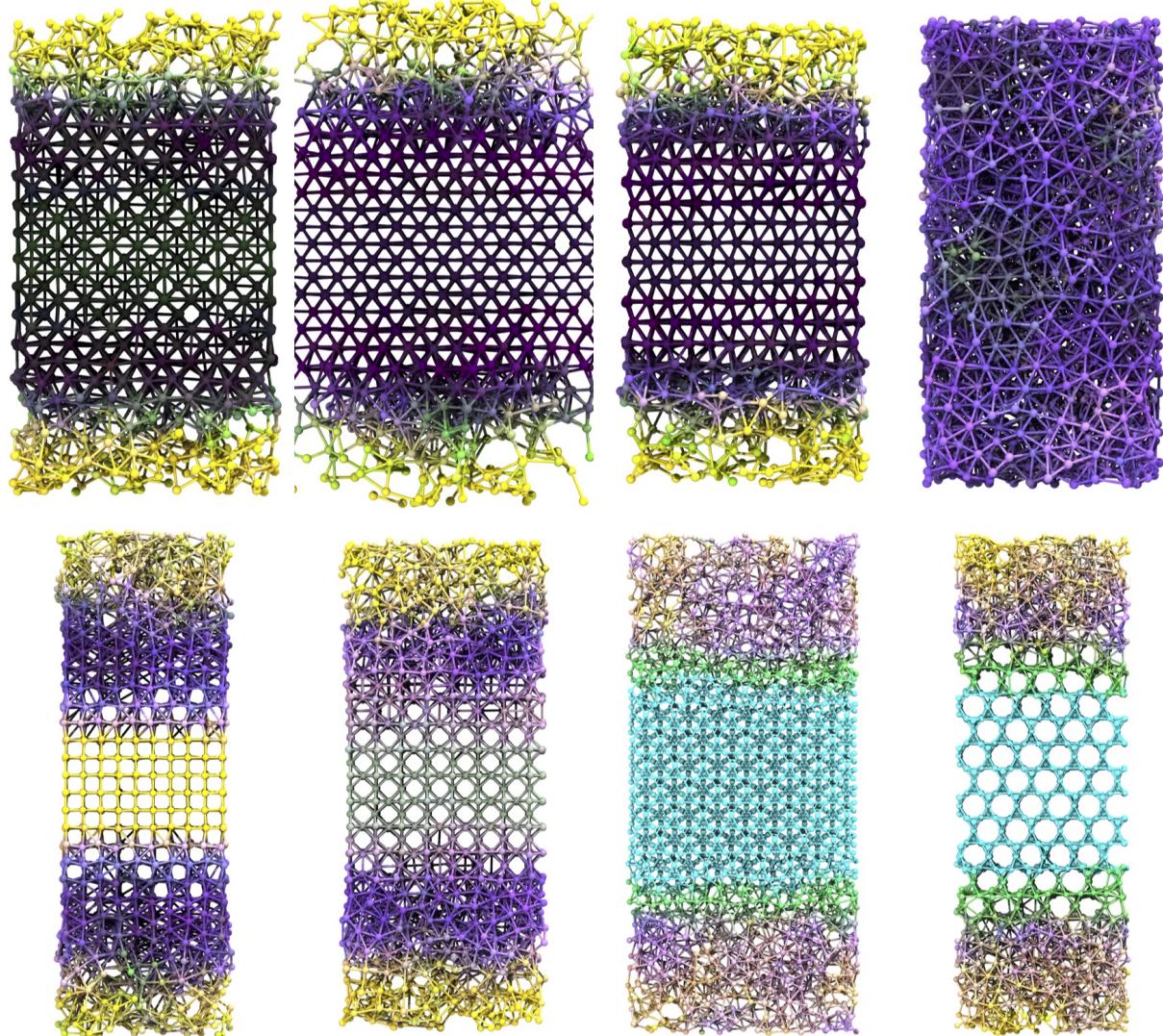


FIG. S2: Snapshots of thermalized crystal lattices colored according to the diffusion map of Fig. 4, built from third-degree neighborhood graphs. Top row: BCC, FCC, HCP, liquid. Bottom row: SC, perovskite, CT, HT.