

Supplementary Information to “Simulating Crystallization in a Colloidal System Using State Predictive Information Bottleneck based Enhanced Sampling”

Vanessa J. Meraz,¹ Ziyue Zou,² and Pratyush Tiwary^{1,2,3,*}

¹*Institute for Physical Science and Technology, University of Maryland, College Park 20742, USA.*

²*Department of Chemistry and Biochemistry, University of Maryland, College Park 20742, USA.*

³*University of Maryland Institute for Health Computing, Rockville 20852, USA.*

arXiv:2404.17722v1 [cond-mat.soft] 26 Apr 2024

* ptiwary@umd.edu

S1. METADYNAMICS TRAJECTORIES

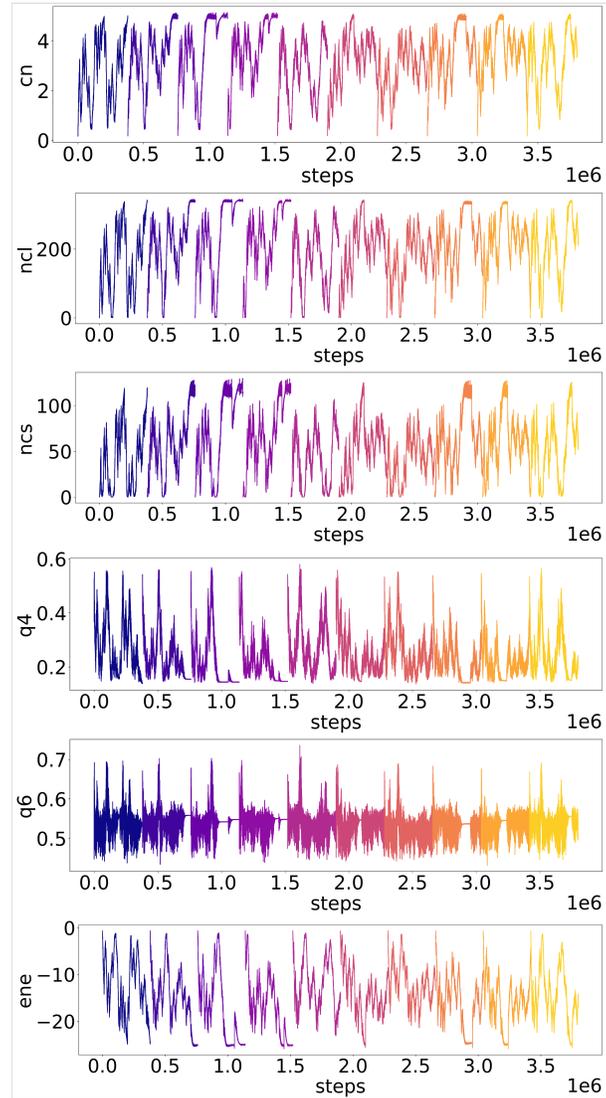


FIG. S1: Each row shows an order parameter plot for 10 concatenated metadynamics trajectories discretized by color. As mentioned in the main text, there is clear back-and-forth movement between phases seen clearly several OPs. Within their respective plots, we can note the dense crystal phase formation briefly in a couple of trajectories where $cn > 4$ or $ene < -20\epsilon$.

S2. ORDER PARAMETER HISTOGRAMS

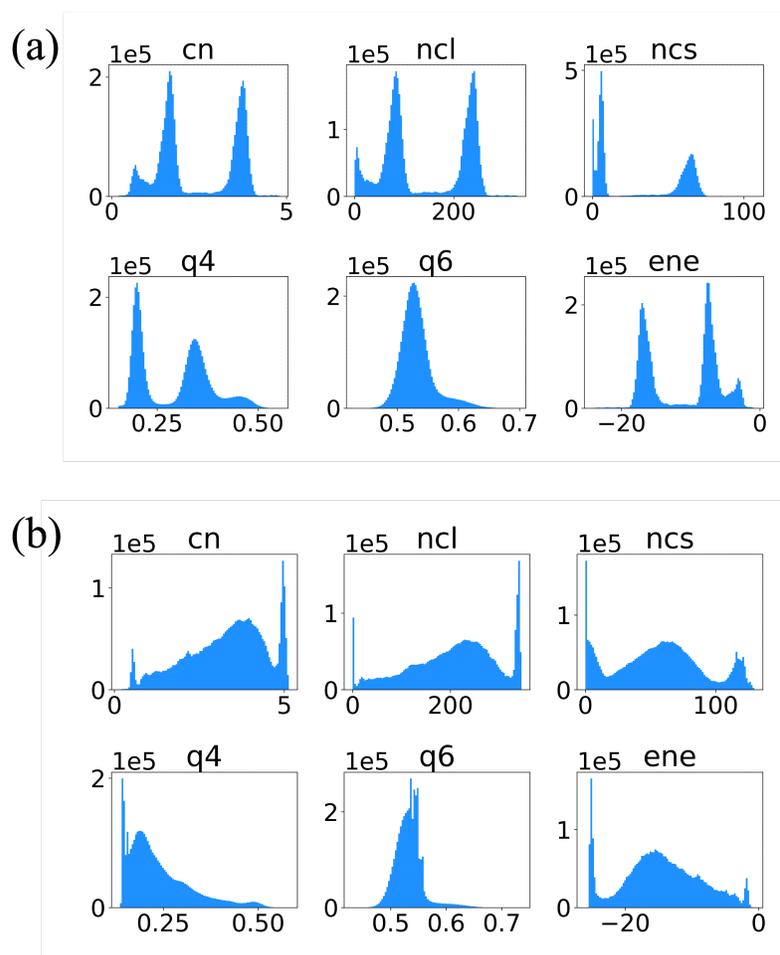


FIG. S2: In this figure we provide for the sake of completeness direct histograms for different OPs (without any correction for biasing) from (a) unbiased simulations and (b) biased metadynamics runs.

S3. ONE-DIMENSIONAL FREE ENERGY PROFILE FOR ALL ORDER PARAMETERS

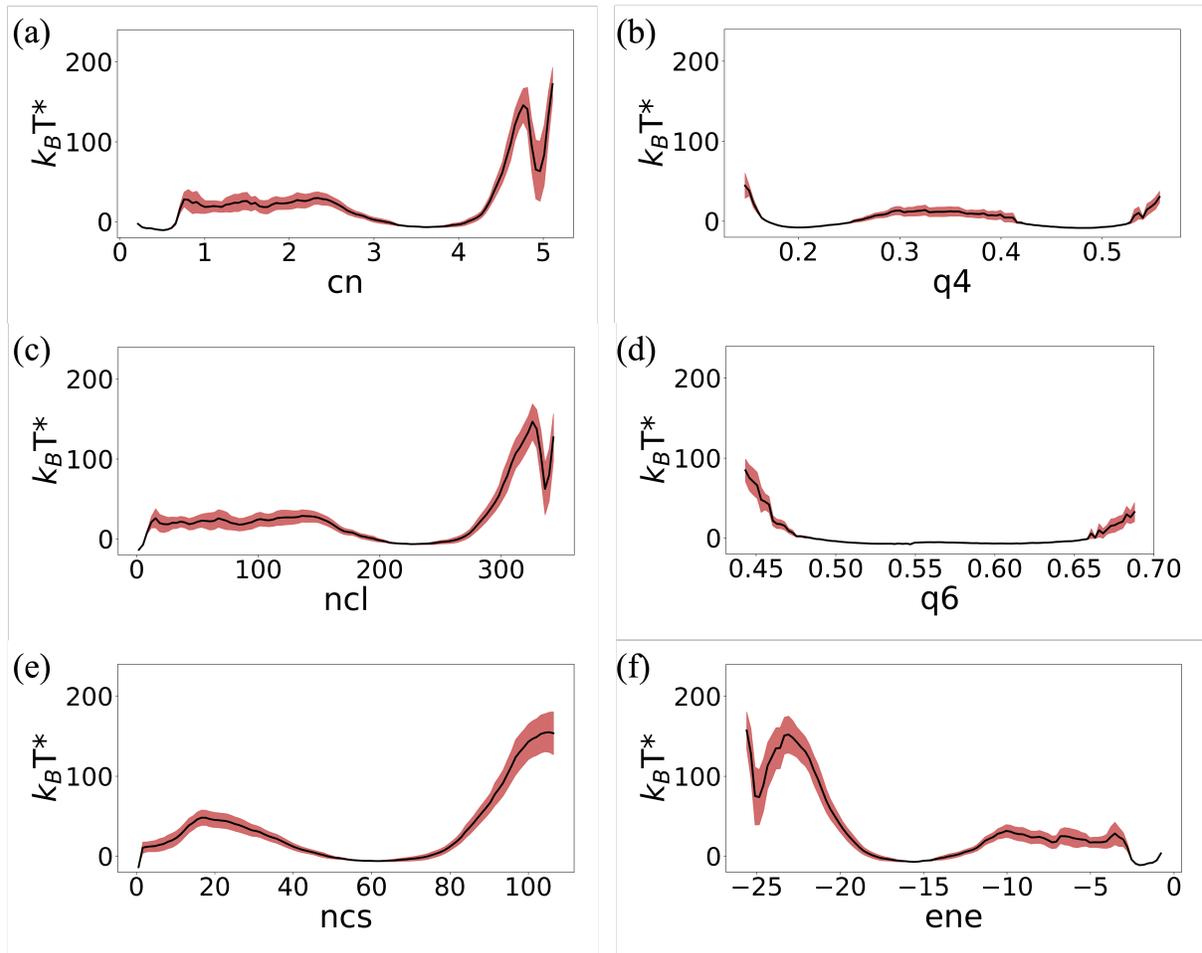


FIG. S3: In this figure we provide one-dimensional free energy profile in units of $k_B T^*$ for each OP. In agreement with Fig. 4 from the main text, which shows the weights of the OPs from the learned SPIB RC, we can observe similarities in the structure of the SPIB z coordinate free energy profile shown in Fig. 8 and the individual ones plotted here. We highlight that the two highest contributors to the RC, the mean coordination number (cn) and the number of particles in a solid-like phase (ncs), have similar features in their free energy profile to that of z . Notably, (e) is missing the well characteristic of the dense crystal phase which is otherwise seen in (a), (c), and (f).

S4. PAIR-PLOTS FOR TWO-DIMENSIONAL FREE ENERGY PROJECTIONS

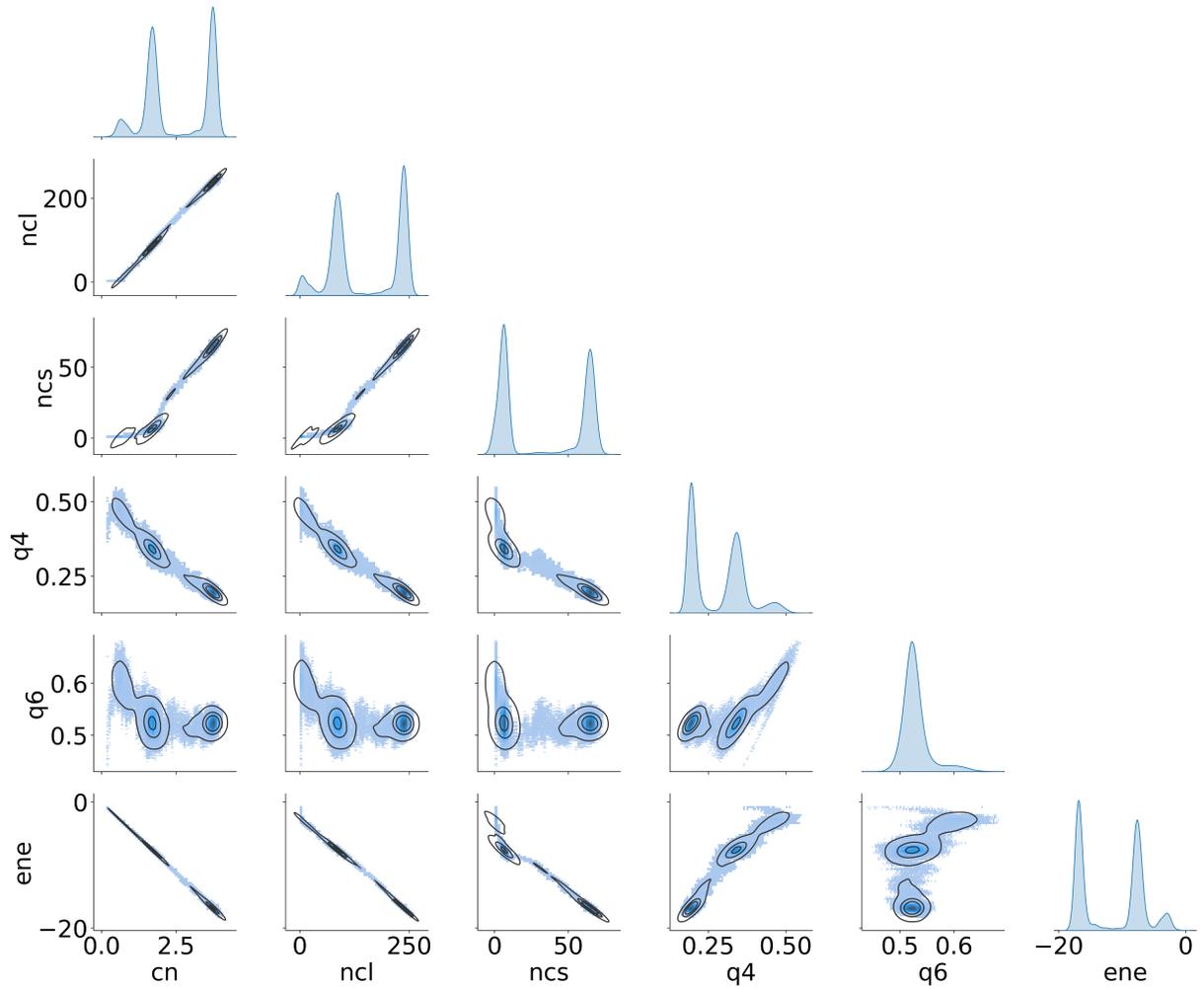


FIG. S4: As an aid to pick the best representation of a two-dimensional free energy landscape, the pair-plot generated by seaborn in Fig. S4 was used. Seemingly, quite a few order parameters are highly correlated which don't allow for an easy insight into the systems' phase. Though not as easy to interpret, Steinhardt bond order parameter q_6 is the most expressive OP, in which three wells to represent the phases of the system can be seen. Hence, the projection onto q_6 and energy is most useful to us and is provided in the main text. Across the diagonal of Fig. S4 are kernel density estimations (KDEs) for the respective column-wise OP. These are also analogous to the histograms shown in Fig. S2(a). Overlaid on the blue tinted histogram plots in the lower triangle shown in black lines are KDEs.