chair planar half-chair boat twist-boat

Energy Profile of the Simulations
color corresponds to the initial conformer of the simuation

(a)

Energy

Simulation Timestep
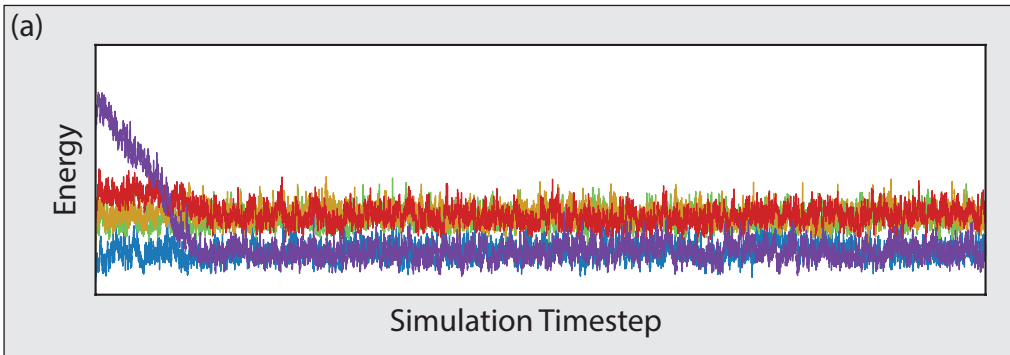
Projections of Simulation Frames
color corresponds to the most similar conformer

(b) PC_2 / PC_1

(c) $KPCA_2$ / $KPCA_1$

(d) $t-SNE_2$ / $t-SNE_1$

(e) $UMAP_2$ / $UMAP_1$