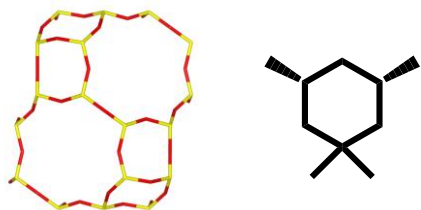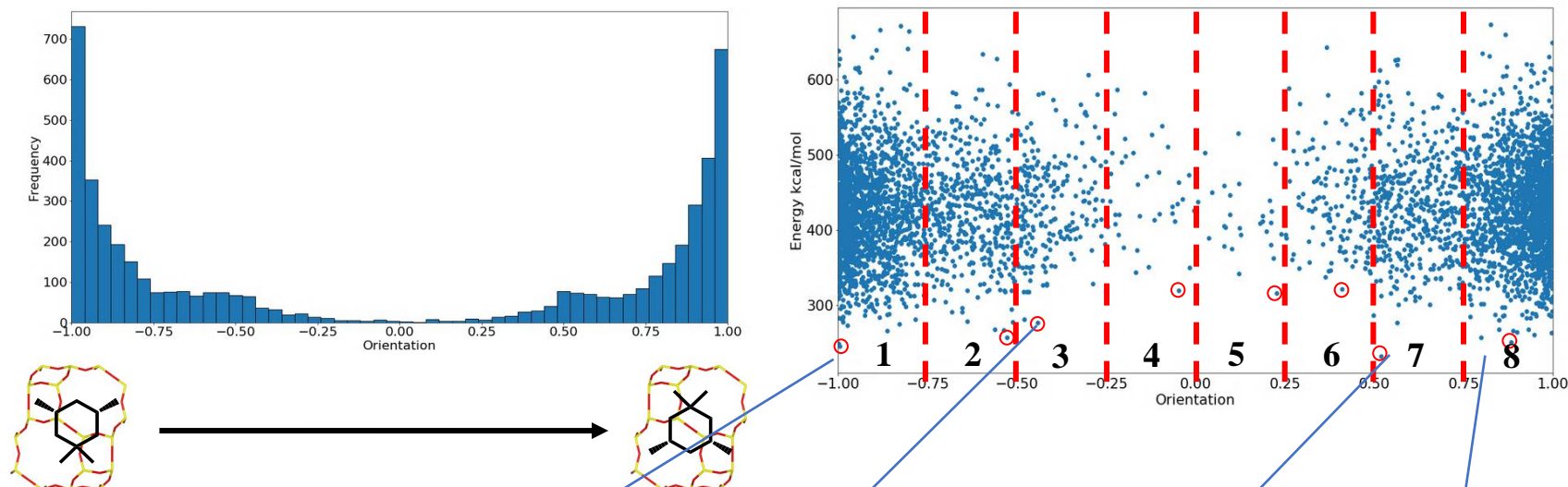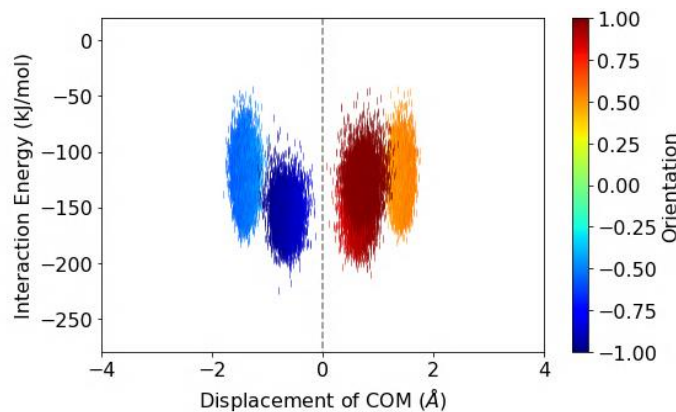1. Insert one OSDA into zeolite cage with random location and orientation and sample with MD under 5000 K for 1 million fs equilibration run and 1 million fs production run.

2. Plot orientation(cos) vs PE for each image in 5000 K MD trajectory. Equally divide the data into 8 bins by their spatial cosine value and choose the lowest energy structure as the representative and resample them at 343 K with MD.

Resample with MD at 343 K

3. Plot orientation vs displacement vs IE for each low temperature MD trajectory.