Supplementary Information

Stepwise kinetics of the Early-Stage Nucleation in Chiral Perovskites via Ab Initio Molecular Dynamics and Free-Energy Simulations

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Table S1. Potential energy values calculated by averaging the potential energy across various configurations at fixed RMSD values and predicted through single point PBE-D3 calculations.

RMSD (Å)	Averaged potential energy (Ry)	$\Delta E_{average}$ (kcal/mol)	Single point potential energy (Ry)	$\Delta ES_{SinglePoint}$ (kcal/mol)
0.0	-1074.223541	0.0	-1074.249425	0.0
0.5	-1074.155852	21.2	-1074.155335	29.5
1.0	-1074.052601	53.6	-1074.040737	65.5
1.5	-1074.083856	43.8	-1074.083856	50.2
2.0	-1073.981819	74.8	-1074.006880	76.1
2.5	-1074.006880	69.8	-1074.006880	73.0
3.0	-1074.060389	50.1	-1074.051717	62.0

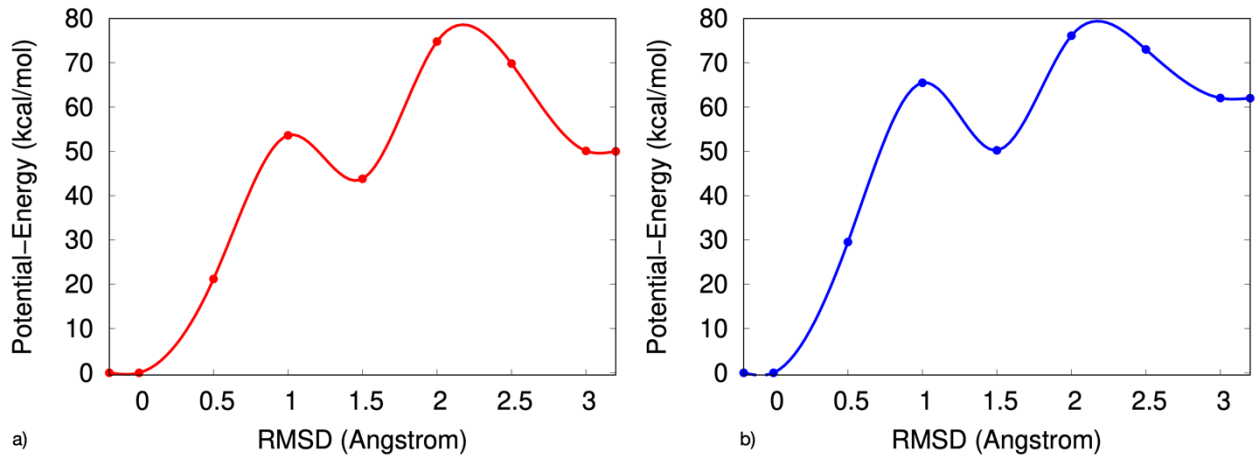

Figure S1. a) The potential energy surface as a function of the RMSD value, calculated by averaging the potential energy across configurations of the system at fixed RMSD values. b) Single point PBE-D3 calculations on configurations at fixed RMSD values.