

Supporting Information for

Utilizing Machine Learning to Greatly Expand the Range and Accuracy of Bottom-Up Coarse-Grained Models Through Virtual Particles

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Description of Machine-Learned Model Features

As discussed in the main text, features for each machine-learned model consisted of binned statistics of pairwise nonbonded, bonded, and angular interactions, as well as pairwise moments for all interactions. For nonbonded interaction bins, the bin width was set to 0.1 Å for all bins and the outer range for each bin was the pair cutoff of 25 Å. Inner cutoffs were chosen individually through analysis of pairwise statistics. Bonded and angular bins used a bin width of 0.05 Å and 5°, respectively. We list bin ranges for all interactions in Tables S1 and S2.

Table S1. Bin ranges for nonbonded and bonded pair interactions.

Interaction Type	Type 1	Type 2	Inner Cutoff (Å)	Outer Cutoff (Å)
Nonbonded	HG	HG	4.0	25.0
	HG	MG	4.0	25.0
	HG	T1	5.5	25.0
	HG	T2	7.6	25.0
	MG	MG	4.0	25.0
	MG	T1	4.0	25.0
	MG	T2	4.9	25.0
	T1	T1	3.4	25.0
	T1	T2	3.4	25.0
	T2	T2	3.4	25.0
Bonded	HG	MG	3.25	7.5
	MG	T1	3.5	10.0
	T1	T2	3.25	10.0

Table S2. Bin ranges for angular interactions.

Interaction Type	Type 1	Type 2	Type 3	Inner Cutoff (°)	Outer Cutoff (°)
Angle	HG	MG	T1	40	180
	MG	T1	T2	30	180
	T1	MG	T2	32	179.5

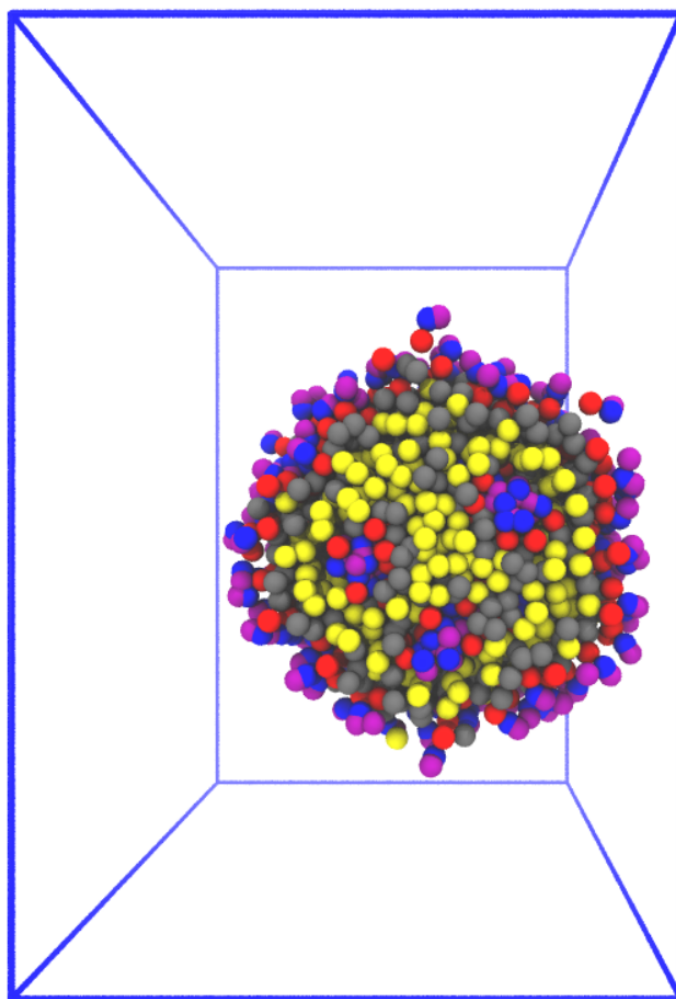


Figure S1. Failure of VD-REM-7 to properly self-assemble into a bilayer configuration when virtual particles are rendered non-interacting. Colors are consistent with the main text.

Movie S1. Self-assembly of VD-REM-7 from a random, dispersed state. xy -dimensions are consistent with reference bilayer area. Simulation occurs over 2×10^6 MD timesteps. Colors are consistent with the main text.