

Universal folding pathways of polyhedron nets: Supplementary Information

Paul M. Dodd^a, Pablo F. Damasceno^b, and Sharon C. Glotzer^{a,b,c,d}

^aChemical Engineering Department, University of Michigan, Ann Arbor, MI 48109, USA; ^bApplied Physics Program, University of Michigan, Ann Arbor, MI 48109, USA; ^cDepartment of Materials Science and Engineering, University of Michigan, Ann Arbor, MI 48109, USA; ^dBiointerfaces Institute, University of Michigan, Ann Arbor, MI 48109, USA

This manuscript was compiled on May 5, 2018

























Image	Database Id	T_m	Diameter	Leaves	Paths
	0	2.50	3	2	2
	1	2.50	2	3	3
	0	4.10	4	3	9
	1	3.57	4	4	12
	2	3.10	4	3	6
	3	4.04	4	3	12
	4	4.16	5	2	6
	5	3.35	3	4	16
	6	4.15	5	2	2
	7	3.95	4	2	6
	8	3.99	5	4	8
	9	3.98	5	3	5
	10	3.74	3	4	18
	0	2.44	6	2	5
	1	2.49	6	3	7
	2	2.48	5	4	12
	3	2.56	7	3	6
	4	2.48	6	3	4
	5	2.49	7	2	6
	6	2.50	5	4	14
	7	2.45	5	3	12
	8	2.47	7	2	2
	9	2.50	5	3	12
	10	2.44	5	2	8

Table S1. Relevant data for the tetrahedron, cube, and octahedron nets. For each net, a database ID, melting temperature T_m , diameter, number of leaves, and number of paths connecting unfolded and folded states is shown.

125
126
127
128
129
130
131
132
133
134
135
136
137
138
139
140
141
142
143
144
145
146
147
148
149
150
151
152
153
154
155
156
157
158
159
160
161
162
163
164
165
166
167
168
169
170
171
172
173
174
175
176
177
178
179
180
181
182
183
184
185
186

187
188
189
190
191
192
193
194
195
196
197
198
199
200
201
202
203
204
205
206
207
208
209
210
211
212
213
214
215
216
217
218
219
220
221
222
223
224
225
226
227
228
229
230
231
232
233
234
235
236
237
238
239
240
241
242
243
244
245
246
247
248

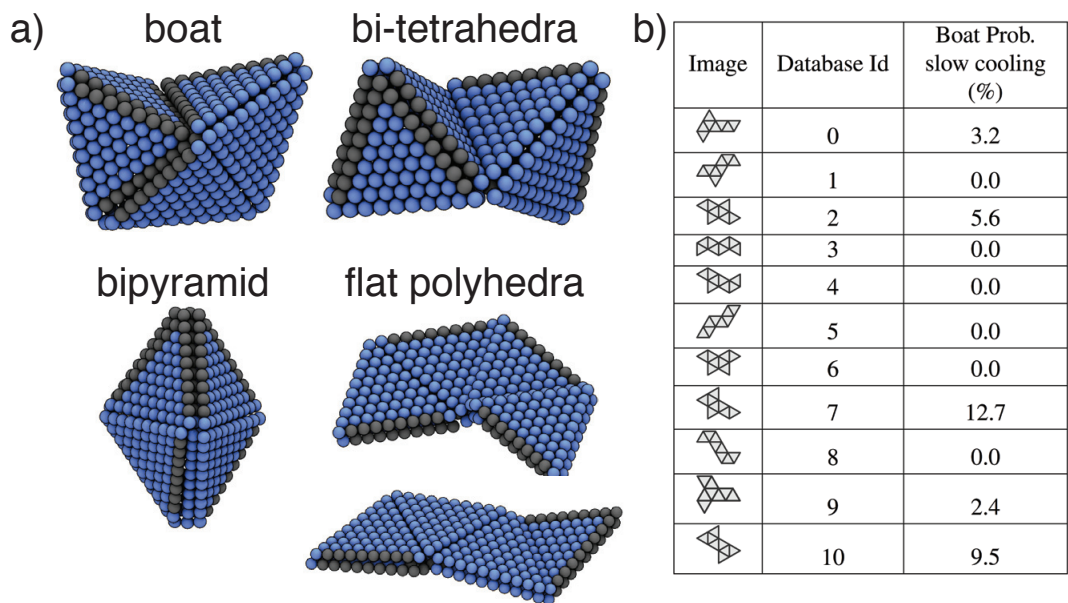


Fig. S1. Octahedron net misfolds. (a) Examples of trapped states that can be achieved by octahedron nets. The boat conformation occurs more often. (b) Probabilities of the octahedron nets folding into the boat conformation for the slow ($2.5 \times 10^{-8} T/t$) cooling rate.

249
250
251
252
253
254
255
256
257
258
259
260
261
262
263
264
265
266
267
268
269
270
271
272
273
274
275
276
277
278
279
280
281
282
283
284
285
286
287
288
289
290
291
292
293
294
295
296
297
298
299
300
301
302
303
304
305
306
307
308
309
310

311
312
313
314
315
316
317
318
319
320
321
322
323
324
325
326
327
328
329
330
331
332
333
334
335
336
337
338
339
340
341
342
343
344
345
346
347
348
349
350
351
352
353
354
355
356
357
358
359
360
361
362
363
364
365
366
367
368
369
370
371
372

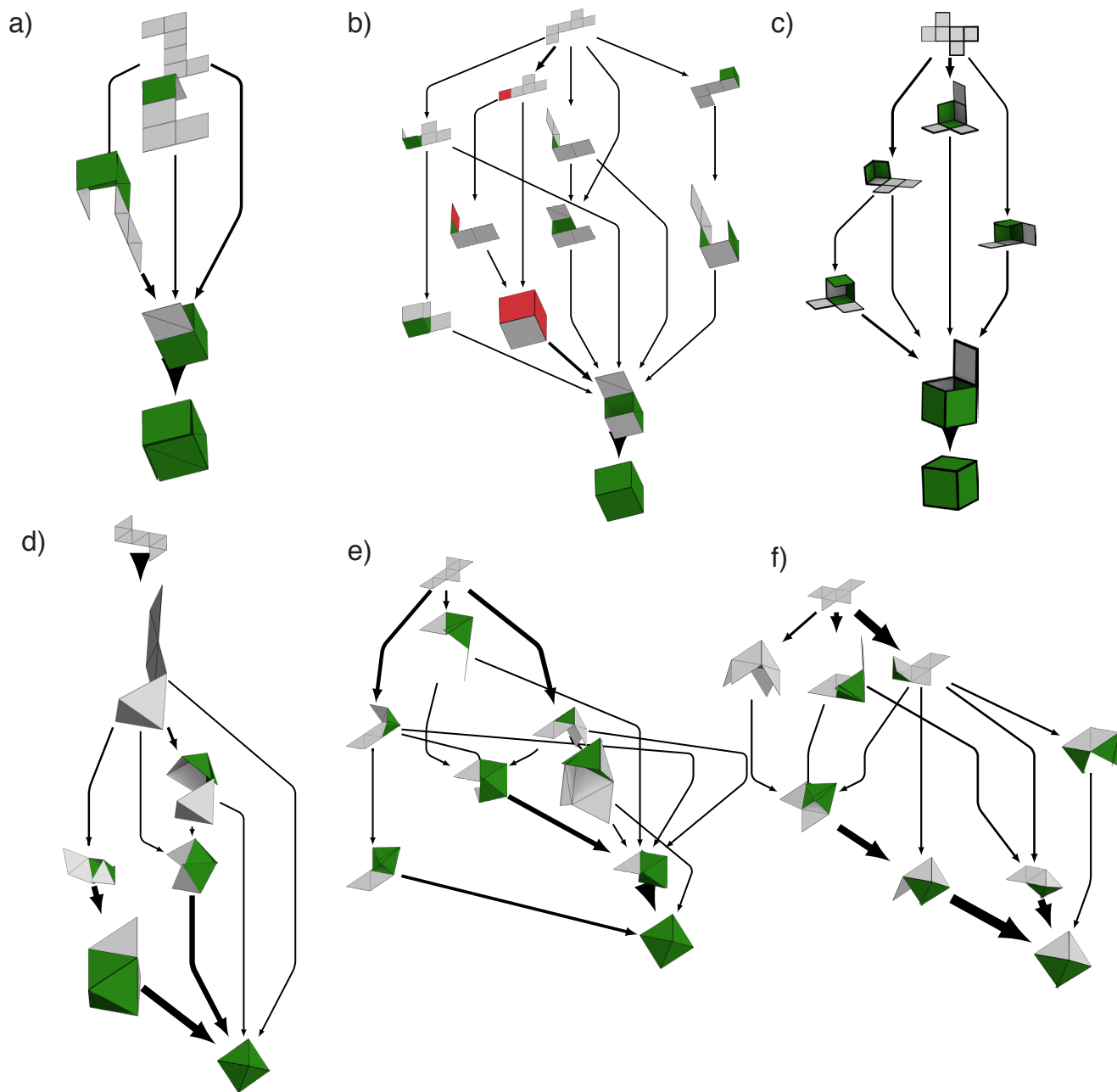


Fig. S2. Folding networks for representative cube and octahedron nets that have two (a,d), three (b,e), and four leaves (c,f). Networks were calculated at the melting temperature reported in Table S1.

373
374
375
376
377
378
379
380
381
382
383
384
385
386
387
388
389
390
391
392
393
394
395
396
397
398
399
400
401
402
403
404
405
406
407
408
409
410
411
412
413
414
415
416
417
418
419
420
421
422
423
424
425
426
427
428
429
430
431
432
433
434

435
436
437
438
439
440
441
442
443
444
445
446
447
448
449
450
451
452
453
454
455
456
457
458
459
460
461
462
463
464
465
466
467
468
469
470
471
472
473
474
475
476
477
478
479
480
481
482
483
484
485
486
487
488
489
490
491
492
493
494
495
496

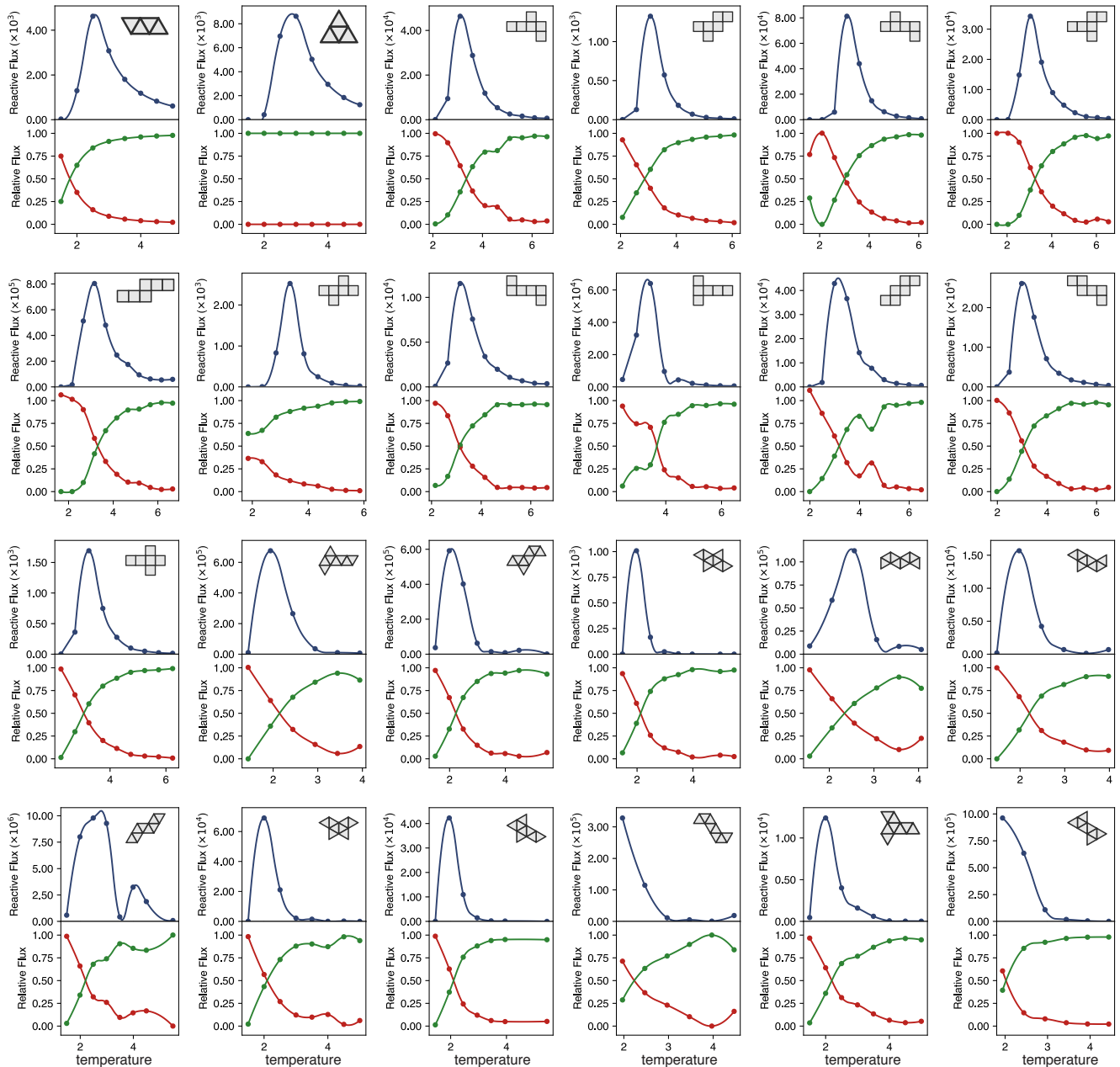


Fig. S3. Temperature dependence of reactive and relative fluxes for the tetrahedron, cube, and octahedron nets. The net corresponding to each plot is given as an inset. For each plot the blue curve represents the total reactive flux while the red and green curves represent the fraction of the flux corresponding to non-native and native contacts, respectively.

497
498
499
500
501
502
503
504
505
506
507
508
509
510
511
512
513
514
515
516
517
518
519
520
521
522
523
524
525
526
527
528
529
530
531
532
533
534
535
536
537
538
539
540
541
542
543
544
545
546
547
548
549
550
551
552
553
554
555
556
557
558

559
560
561
562
563
564
565
566
567
568
569
570
571
572
573
574
575
576
577
578
579
580
581
582
583
584
585
586
587
588
589
590
591
592
593
594
595
596
597
598
599
600
601
602
603
604
605
606
607
608
609
610
611
612
613
614
615
616
617
618
619
620

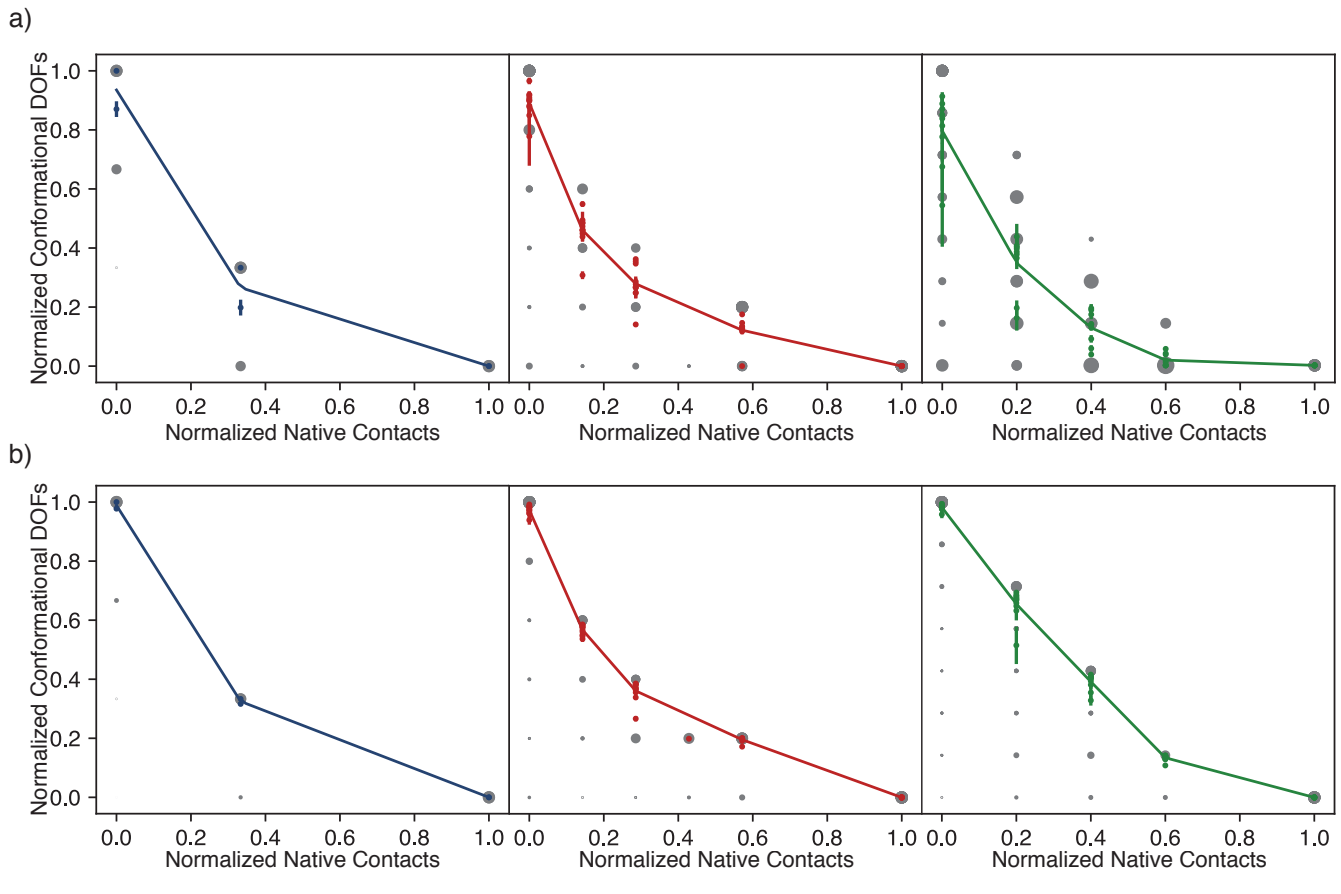


Fig. S4. The normalized conformational degrees of freedom of each net for the tetrahedron (blue), cube (red), and octahedron (green), as a function of the normalized number of native contacts for two different temperature regimes. All pathways from all net are projected onto this plot. Each gray point represents an intermediate observed in a reactive pathway and the size of each point is proportional to the probability that intermediate is in a reactive pathway. a) Pathways observed for a temperatures lower than the crossover temperature ($T = T_m - 1$). b) Pathways observed for a temperatures greater than the crossover temperature ($T = T_m + 0.5$). We find no correlation between the folding propensity and the proximity to the diagonal line at high temperature.

621
622
623
624
625
626
627
628
629
630
631
632
633
634
635
636
637
638
639
640
641
642
643
644
645
646
647
648
649
650
651
652
653
654
655
656
657
658
659
660
661
662
663
664
665
666
667
668
669
670
671
672
673
674
675
676
677
678
679
680
681
682

683
684
685
686
687
688
689
690
691
692
693
694
695
696
697
698
699
700
701
702
703
704
705
706
707
708
709
710
711
712
713
714
715
716
717
718
719
720
721
722
723
724
725
726
727
728
729
730
731
732
733
734
735
736
737
738
739
740
741
742
743
744

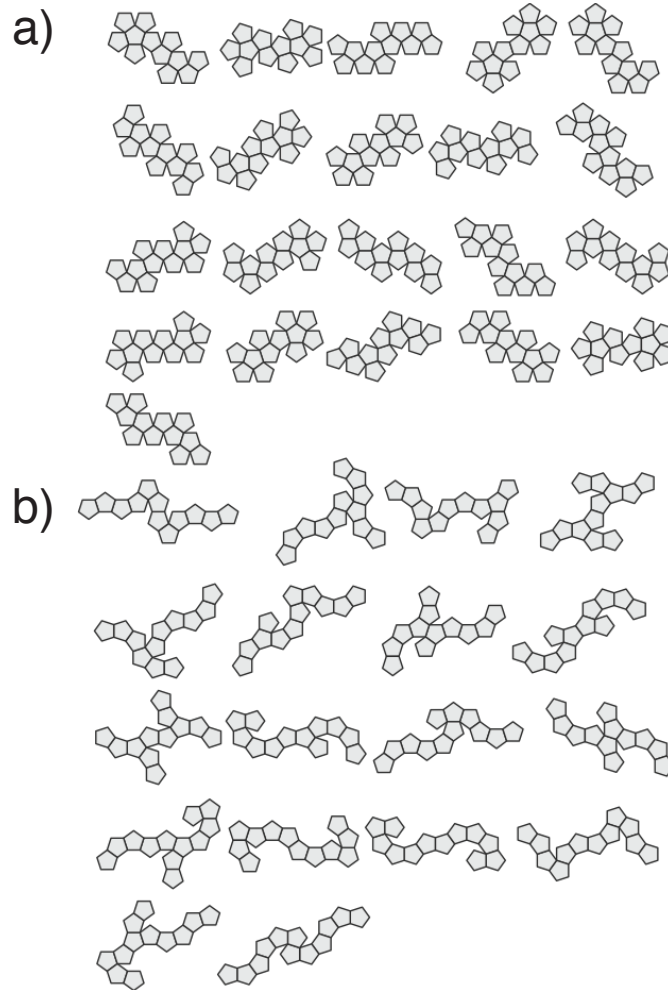


Fig. S5. Dodecahedron nets used in this study. Dodecahedron nets predicted to be "good" (a) folders and "bad" (b) folders.

745
746
747
748
749
750
751
752
753
754
755
756
757
758
759
760
761
762
763
764
765
766
767
768
769
770
771
772
773
774
775
776
777
778
779
780
781
782
783
784
785
786
787
788
789
790
791
792
793
794
795
796
797
798
799
800
801
802
803
804
805
806

807
808
809
810
811
812
813
814
815
816
817
818
819
820
821
822
823
824
825
826
827
828
829
830
831
832
833
834
835
836
837
838
839
840
841
842
843
844
845
846
847
848
849
850
851
852
853
854
855
856
857
858
859
860
861
862
863
864
865
866
867
868

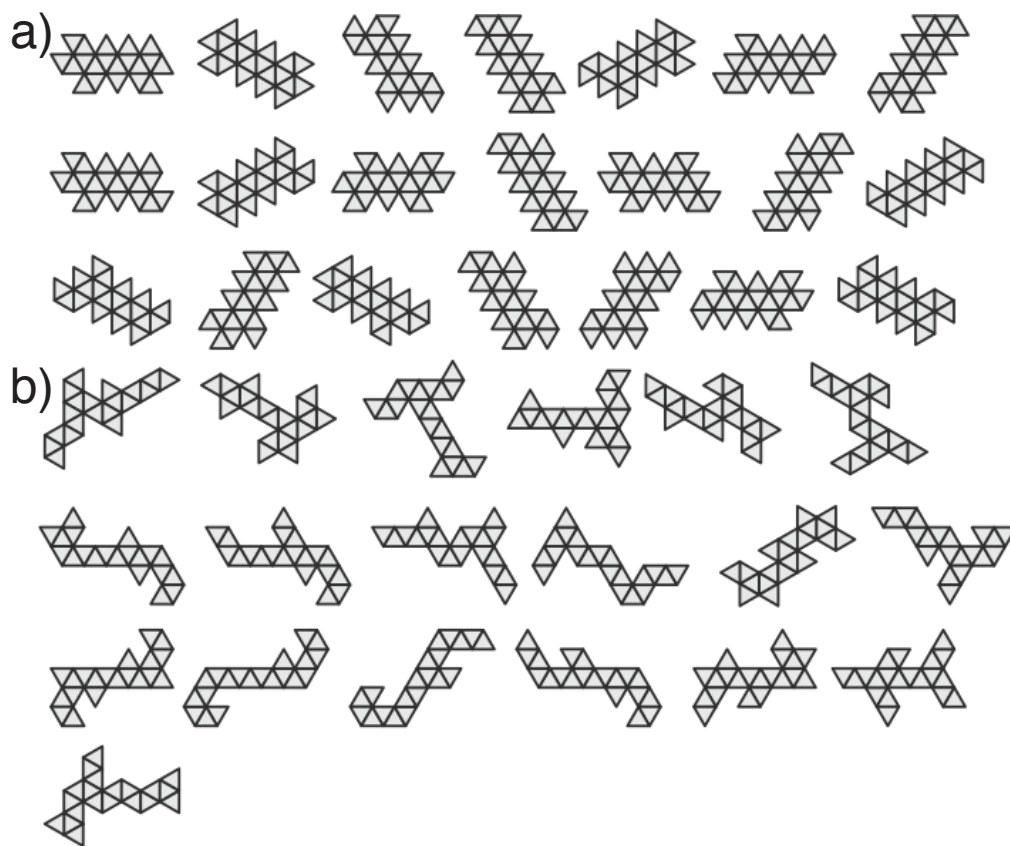


Fig. S6. Icosahedron nets used in this study. Icosahedron nets predicted to be "good" (a) folders and "bad" (b) folders.

869
870
871
872
873
874
875
876
877
878
879
880
881
882
883
884
885
886
887
888
889
890
891
892
893
894
895
896
897
898
899
900
901
902
903
904
905
906
907
908
909
910
911
912
913
914
915
916
917
918
919
920
921
922
923
924
925
926
927
928
929
930

931
932
933
934
935
936
937
938
939
940
941
942
943
944
945
946
947
948
949
950
951
952
953
954
955
956
957
958
959
960
961
962
963
964
965
966
967
968
969
970
971
972
973
974
975
976
977
978
979
980
981
982
983
984
985
986
987
988
989
990
991
992

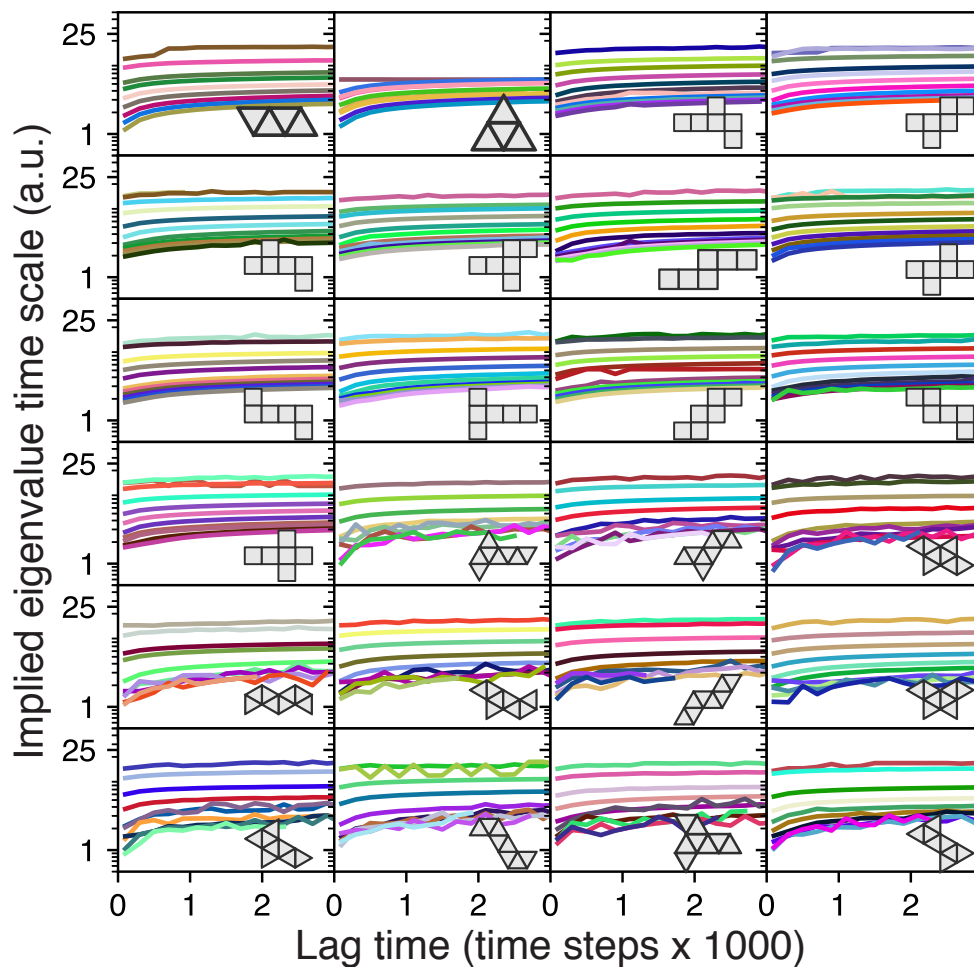


Fig. S7. Choice of lag time for MSM studies. For each tetrahedron, cube, and octahedron net (shown in the inset), the implied time scales is shown. Each curve shows the first non-trivial eigenvalue, λ_2 , of the transition probability matrix, as a function of the lag time, τ , for a given temperature. The colors are random and distinguish different temperatures. All of the eigenvalues flatten out by $\tau = 1000$ time steps. We therefore choose this value as the lag time for each MSM study.

993	1055
994	1056
995	1057
996	1058
997	1059
998	1060
999	1061
1000	1062
1001	1063
1002	1064
1003	1065
1004	1066
1005	1067
1006	1068
1007	1069
1008	1070
1009	1071
1010	1072
1011	1073
1012	1074
1013	1075
1014	1076
1015	1077
1016	1078
1017	1079
1018	1080
1019	1081
1020	1082
1021	1083
1022	1084
1023	1085
1024	1086
1025	1087
1026	1088
1027	1089
1028	1090
1029	1091
1030	1092
1031	1093
1032	1094
1033	1095
1034	1096
1035	1097
1036	1098
1037	1099
1038	1100
1039	1101
1040	1102
1041	1103
1042	1104
1043	1105
1044	1106
1045	1107
1046	1108
1047	1109
1048	1110
1049	1111
1050	1112
1051	1113
1052	1114
1053	1115
1054	1116