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Supporting Information

Langevin dynamics simulations for the critical adsorption of end-grafted active polymers

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1. Supplementary Plots

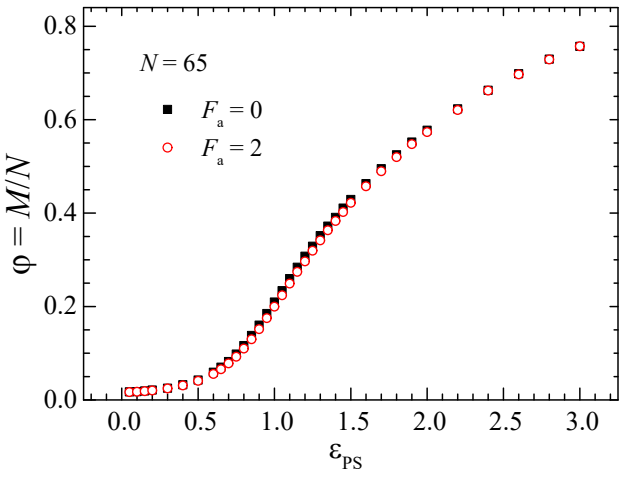

Figure S1. Plots of the fraction of adsorbed monomers φ *versus* the surface attraction strength ε_{PS} for a purely passive polymer ($F_a = 0$) and for the RRAP chain at $F_a = 2$. Polymer length $N = 65$.

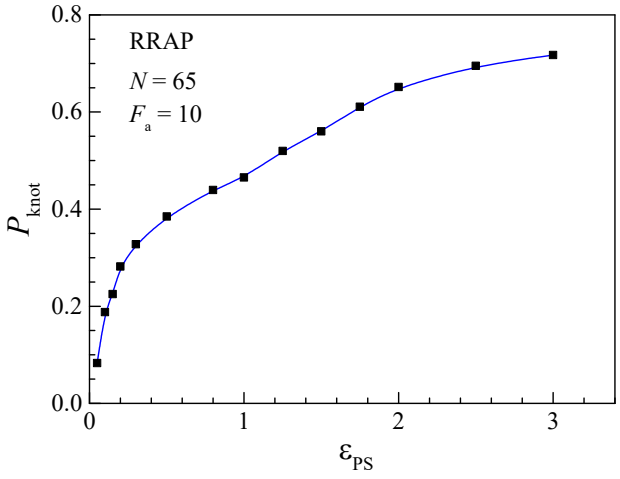

Figure S2. Plots of the probability of knotted conformations, P_{knot}, *versus* the surface

attraction strength ε_{PS} at $F_a = 10$ for the RRAP chain. Polymer length $N = 65$.

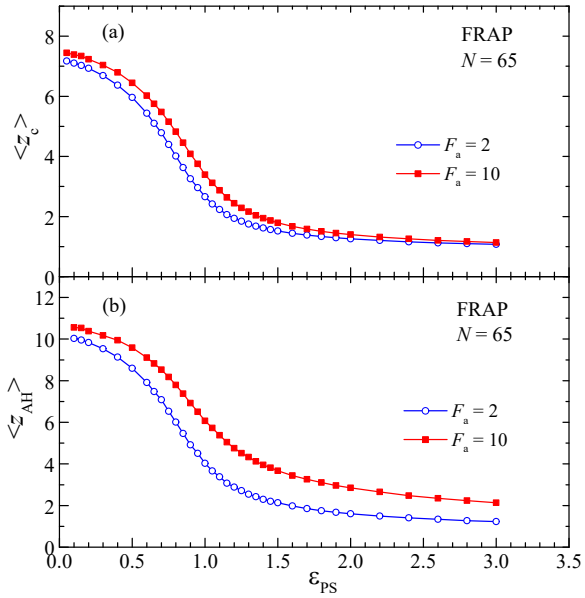

Figure S3. Plot of the mean height of the mass center of chain $<z_c>$ (a) and the mean height of the active head $<z_{AH}>$ (b) *versus* the surface attraction strength ε_{PS} for the FRAP chain with $F_a = 2$ and 10.

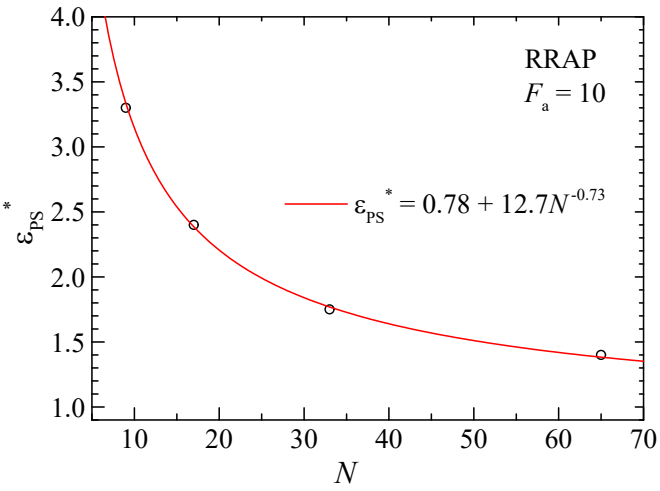

Figure S4. Plot of the critical attraction strength ε_{PS}^* *versus* polymer length for the RRAP chain at the active force $F_a = 10$. The fitting function (solid line) is presented in the plot.

2. Original simulation data

2.1 Figure 2

$F_a = 2$		$F_a = 10$	
ε_{PS}	φ	ε_{PS}	φ
0.05	0.016827	0.05	0.013743
0.1	0.017349	0.1	0.014742
0.15	0.018566	0.15	0.016205
0.2	0.020267	0.2	0.018089
0.3	0.024666	0.3	0.022392
0.4	0.030960	0.4	0.028169
0.5	0.040818	0.5	0.035937
0.6	0.055527	0.6	0.045209
0.65	0.065582	0.7	0.058596
0.7	0.078228	0.8	0.073547
0.75	0.092347	0.9	0.091287
0.8	0.109841	1	0.112402
0.85	0.129731	1.1	0.135957
0.9	0.151458	1.2	0.161146
0.95	0.175172	1.25	0.174940
1	0.199576	1.3	0.187671
1.05	0.223946	1.35	0.201254
1.1	0.248993	1.4	0.214387
1.15	0.274164	1.45	0.227458
1.2	0.296485	1.5	0.240422
1.25	0.319442	1.55	0.254113
1.3	0.341602	1.6	0.265821
1.35	0.363250	1.65	0.277397
1.4	0.383200	1.7	0.290178
1.45	0.402357	1.75	0.301544
1.5	0.422000	1.8	0.313468
1.6	0.457319	1.85	0.324719
1.7	0.489664	1.9	0.334116
1.8	0.519897	1.95	0.344734
1.9	0.547681	2	0.354758
2	0.573334	2.1	0.374130
2.2	0.620658	2.2	0.393701
2.4	0.662192	2.3	0.410950
2.6	0.696843	2.4	0.428787
2.8	0.728832	2.5	0.444496
3	0.757080	2.6	0.458328
		2.8	0.487365
		3	0.514487

		3.2	0.537743
		3.5	0.571526

2.2 Figure 3

$F_a = 2$			$F_a = 10$		
ε_{PS}	z_c	z_{AH}	ε_{PS}	z_c	z_{AH}
0.05	7.288899	10.38655	0.05	9.862102	15.76225
0.1	7.280643	10.39378	0.1	9.555289	15.45045
0.15	7.187031	10.2963	0.15	9.288182	15.17549
0.2	7.091079	10.18016	0.2	9.026822	14.89146
0.3	6.870788	9.956771	0.3	8.734113	14.58075
0.4	6.560311	9.545372	0.4	8.439739	14.30046
0.5	6.18401	9.11836	0.5	8.148983	14.0254
0.6	5.662987	8.468727	0.6	7.855844	13.74791
0.65	5.367629	8.110569	0.7	7.482003	13.3648
0.7	5.013044	7.678966	0.8	7.152283	13.06353
0.75	4.667694	7.226649	0.9	6.788079	12.73831
0.8	4.274289	6.742889	1	6.392645	12.3263
0.85	3.89196	6.223869	1.1	5.99374	11.91371
0.9	3.519174	5.742502	1.2	5.557679	11.41821
0.95	3.160882	5.218263	1.25	5.327621	11.14254
1	2.862689	4.799648	1.3	5.117769	10.89644
1.05	2.61593	4.433515	1.35	4.906686	10.63221
1.1	2.391109	4.087194	1.4	4.710092	10.35238
1.15	2.20179	3.768725	1.45	4.526391	10.12916
1.2	2.063868	3.548524	1.5	4.348683	9.872656
1.25	1.939939	3.329345	1.55	4.146761	9.58579
1.3	1.83842	3.12561	1.6	3.997393	9.380523
1.35	1.751091	2.95027	1.65	3.845666	9.150668
1.4	1.680072	2.818574	1.7	3.694236	8.916982
1.45	1.620757	2.693533	1.75	3.565477	8.71585
1.5	1.567218	2.585875	1.8	3.439334	8.509382
1.6	1.478408	2.37616	1.85	3.320283	8.310033
1.7	1.410551	2.22262	1.9	3.216137	8.118358
1.8	1.356044	2.091053	1.95	3.102682	7.916845
1.9	1.310103	1.964218	2	2.99903	7.714899
2	1.272722	1.869494	2.1	2.818343	7.35445
2.2	1.211561	1.704404	2.2	2.665111	7.049581
2.4	1.165131	1.575867	2.3	2.528812	6.759186
2.6	1.129783	1.477432	2.4	2.395161	6.451998
2.8	1.100024	1.39339	2.5	2.283361	6.15847
3	1.075657	1.322761	2.6	2.182461	5.89607
			2.8	2.015995	5.409032

			3	1.870195	4.950444
			3.2	1.750009	4.510368
			3.5	1.606747	3.922324

2.3 Figure 4

$F_a = 2$		$F_a = 10$	
ε_{PS}	$\langle\cos\theta_F\rangle$	ε_{PS}	$\langle\cos\theta_F\rangle$
0.05	0.009398	0.05	0.067332
0.1	0.011483	0.1	0.068935
0.15	0.01179	0.15	0.073537
0.2	0.015159	0.2	0.077519
0.3	0.015425	0.3	0.080606
0.4	0.020505	0.4	0.087023
0.5	0.021908	0.5	0.088372
0.6	0.026629	0.6	0.095038
0.65	0.030288	0.7	0.100015
0.7	0.035103	0.8	0.106052
0.75	0.036085	0.9	0.113697
0.8	0.046493	1	0.123465
0.85	0.049579	1.1	0.129539
0.9	0.057724	1.2	0.138189
0.95	0.062273	1.25	0.143705
1	0.067726	1.3	0.146802
1.05	0.075505	1.35	0.155982
1.1	0.082396	1.4	0.157702
1.15	0.089745	1.45	0.164239
1.2	0.097795	1.5	0.166417
1.25	0.102815	1.55	0.172348
1.3	0.106982	1.6	0.176235
1.35	0.108518	1.65	0.183009
1.4	0.113819	1.7	0.187748
1.45	0.118542	1.75	0.193533
1.5	0.120691	1.8	0.196301
1.6	0.125179	1.85	0.20053
1.7	0.12974	1.9	0.20169
1.8	0.131812	1.95	0.206506
1.9	0.1323	2	0.211408
2	0.133351	2.1	0.216363
2.2	0.13481	2.2	0.225222
2.4	0.131148	2.3	0.229136
2.6	0.128298	2.4	0.234829
2.8	0.121374	2.5	0.239325
3	0.115601	2.6	0.243151

		2.8	0.250845
		3	0.254032
		3.2	0.256282
		3.5	0.252127

2.4 Figure 5

mean adsorption probability P_{ads} for each monomer

monomer index	P_{ads} of $F_a = 2$	P_{ads} of $F_a = 10$
1	0.620013	0.236281
2	0.690563	0.265563
3	0.747063	0.295163
4	0.770638	0.322706
5	0.782138	0.344525
6	0.78435	0.3637
7	0.781025	0.379238
8	0.77795	0.398756
9	0.779475	0.419288
10	0.774738	0.440963
11	0.77785	0.464088
12	0.7749	0.481656
13	0.776	0.498475
14	0.773363	0.510575
15	0.773688	0.5211
16	0.775013	0.533375
17	0.773463	0.54205
18	0.772288	0.54875
19	0.772575	0.55345
20	0.772813	0.560881
21	0.772588	0.572513
22	0.770038	0.577456
23	0.774475	0.582175
24	0.773825	0.579188
25	0.773338	0.577419
26	0.7723	0.579338
27	0.770563	0.580225
28	0.772425	0.582838
29	0.768638	0.581219
30	0.770838	0.577938
31	0.7712	0.573394
32	0.772688	0.572863
33	0.7748	0.575175
34	0.772513	0.58045
35	0.770475	0.5826

36	0.76925	0.58295
37	0.771138	0.580688
38	0.770663	0.579775
39	0.772125	0.577113
40	0.773538	0.577419
41	0.774363	0.577819
42	0.770925	0.577063
43	0.769738	0.576238
44	0.770913	0.580313
45	0.767888	0.583419
46	0.771488	0.584581
47	0.771263	0.5877
48	0.769838	0.590769
49	0.767813	0.596606
50	0.768263	0.602788
51	0.772525	0.610419
52	0.7709	0.609938
53	0.770463	0.59805
54	0.7737	0.582406
55	0.774188	0.573075
56	0.7709	0.592006
57	0.770863	0.631856
58	0.7734	0.666969
59	0.771063	0.666256
60	0.76925	0.591225
61	0.771113	0.452519
62	0.769025	0.271563
63	0.769725	0.232956
64	0.793275	0.251831
65	1	1

2.5 Figure 6

F_a	P_{knot}
1	0
2	0
3	0
4	0.05
5	0.1617
6	0.3728
7	0.6667
8	0.7138
9	0.7684
10	0.7174

12	0.6676
15	0.4274
20	0.1064

2.6 Figure 7

monomer index	P_{ads} of unknotted polymer	P_{ads} of knotted polymer
1	0.21391	0.24509
2	0.24443	0.27389
3	0.27491	0.30314
4	0.30768	0.32863
5	0.33579	0.34797
6	0.36474	0.36329
7	0.38981	0.37507
8	0.41836	0.39103
9	0.4468	0.40845
10	0.47053	0.42931
11	0.50171	0.44926
12	0.52496	0.4646
13	0.55118	0.47771
14	0.57314	0.48593
15	0.5988	0.49049
16	0.61793	0.50007
17	0.6384	0.50409
18	0.65519	0.50682
19	0.67021	0.50745
20	0.68299	0.51278
21	0.70108	0.52186
22	0.7122	0.52437
23	0.7243	0.52618
24	0.73038	0.51962
25	0.74018	0.5133
26	0.75172	0.51143
27	0.75364	0.51191
28	0.76302	0.51185
29	0.76605	0.5084
30	0.77147	0.50169
31	0.77518	0.4939
32	0.776	0.49283
33	0.78038	0.49433
34	0.7867	0.49919
35	0.78345	0.50347
36	0.78626	0.50285

37	0.78847	0.49883
38	0.79228	0.49606
39	0.79024	0.49315
40	0.79336	0.49235
41	0.79341	0.49289
42	0.79004	0.49316
43	0.79139	0.49148
44	0.79449	0.49594
45	0.79307	0.50082
46	0.7936	0.50223
47	0.79073	0.50771
48	0.79358	0.51087
49	0.79433	0.51871
50	0.7936	0.52761
51	0.79427	0.53799
52	0.7967	0.53636
53	0.7915	0.52184
54	0.79321	0.49936
55	0.79128	0.48711
56	0.79292	0.51285
57	0.79299	0.56838
58	0.79343	0.61715
59	0.78945	0.61772
60	0.7921	0.51209
61	0.78923	0.31987
62	0.78794	0.06813
63	0.79243	0.01255
64	0.80798	0.03273
65	1	1

2.7 Figure 8

RRAP			FRAP		
F_a	ε_{PS}^*	Error bat	F_a	ε_{PS}^*	Error bat
0	1.05	0.05	0	1.05	0.05
1	1.05	0.05	2	1.05	0.05
2	1.1	0.05	5	1.1	0.05
3	1.1	0.05	10	1.1	0.05
4	1.15	0.05	15	1.15	0.1
5	1.2	0.05	17	1.2	0.1
6	1.25	0.05	20	1.25	0.1
7	1.25	0.05			
10	1.4	0.1			
12	1.5	0.1			

15	1.95	0.1			
20	2.4	0.1			

2.8 Figure 9

RRAP				FRAP			
ε_{PS}	$\langle\cos\theta_F\rangle$ at $F_a = 10$	ε_{PS}	$\langle\cos\theta_F\rangle$ at $F_a = 20$	ε_{PS}	$\langle\cos\theta_F\rangle$ at $F_a = 10$	ε_{PS}	$\langle\cos\theta_F\rangle$ at $F_a = 20$
0.1	0.06894	0.1	0.20248	0.1	-3.31024E-4	0.1	-9.66758E-4
0.15	0.07354	0.2	0.20232	0.15	-7.86045E-4	0.2	7.36562E-4
0.2	0.07752	0.3	0.20607	0.2	0.00289	0.4	-0.00343
0.3	0.08061	0.4	0.20874	0.3	-6.36557E-4	0.6	-1.40996E-4
0.4	0.08702	0.5	0.20875	0.4	-0.00221	0.8	0.00111
0.5	0.08837	0.6	0.21035	0.5	-8.47294E-4	1	5.4115E-5
0.6	0.09504	0.7	0.21329	0.6	0.00193	1.1	-0.00266
0.7	0.10002	0.8	0.21445	0.65	-0.0011	1.2	-0.00262
0.8	0.10605	0.9	0.21624	0.7	-0.00325	1.3	-0.00535
0.9	0.1137	1	0.21844	0.75	0.00125	1.35	0.00281
1	0.12347	1.1	0.22279	0.8	3.77149E-4	1.4	-0.00189
1.1	0.12954	1.2	0.22499	0.85	-0.00103	1.45	9.20689E-4
1.2	0.13819	1.3	0.22768	0.9	0.00106	1.5	-0.00216
1.25	0.14371	1.4	0.23046	0.95	-0.00211	1.55	-0.0048
1.3	0.1468	1.5	0.235	1	0.00271	1.6	-4.34623E-4
1.35	0.15598	1.6	0.237	1.05	0.00387	1.65	-0.00203
1.4	0.1577	1.7	0.24297	1.1	-7.18952E-4	1.7	0.00505
1.45	0.16424	1.8	0.24784	1.15	0.00173	1.75	0.00456
1.5	0.16642	1.9	0.24978	1.2	3.88977E-4	1.85	0.00468
1.55	0.17235	1.95	0.25291	1.25	-0.00183	2	0.00368
1.6	0.17624	2	0.2556	1.3	0.0017	2.25	0.00505
1.65	0.18301	2.05	0.25651	1.35	2.18291E-4	2.5	0.00472
1.7	0.18775	2.1	0.2581	1.4	0.00213	2.75	0.00683
1.75	0.19353	2.15	0.25969	1.45	0.00206	3	0.00585
1.8	0.1963	2.2	0.26028	1.5	7.9442E-5		
1.85	0.20053	2.25	0.26438	1.6	3.29919E-4		
1.9	0.20169	2.3	0.26383	1.7	0.00285		
1.95	0.20651	2.4	0.2692	1.8	-0.00123		
2	0.21141	2.5	0.27434	1.9	5.34838E-4		
2.1	0.21636	2.6	0.27601	2	-7.17618E-4		
2.2	0.22522	2.7	0.2791	2.2	-5.72747E-4		
2.3	0.22914	2.8	0.28507	2.4	-0.00144		
2.4	0.23483	3	0.29108	2.6	-2.61303E-4		
2.5	0.23933			2.8	5.8223E-4		
2.6	0.24315			3	7.07502E-4		
2.8	0.25084						

3	0.25403						

2.9 Figure 10

	RRAP		FRAP	
N	ε_{PS}^*	Error bar	ε_{PS}^*	Error bar
9	2	0.05	1.3	0.05
17	1.7	0.05	1.25	0.05
33	1.4	0.05	1.15	0.05
65	1.2	0.05	1.1	0.05