

**Towards Hybrid Quantum Mechanical/Molecular
Mechanical Simulations of Li and Na Intercalation in
Graphite - Force Field Development and DFTB
Parametrisation
Supplementary Information**

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S1 Slater-Koster Table Creation - Details

Figure S1 displays a comparison between the original C-C Slater-Koster table and the recreation carried out in this work. Note that the single deviating line is not actually deviating and only a result of the program-immanent conventions as only the absolute values of Hamiltonian and overlap stored in the Slater-Koster table are relevant. Inverting the sign would lead to a corresponding identical line. The Hubbard derivative of sodium deviates by 0.0001 from the respective 3ob value, which is probably a result of employing a different parametrisation software and the influence on the calculation likely is negligible. In general, the generated one-center parameters are comparable with data from previous work of Wahiduzzaman et al.^[1] The observed good agreement confirms that the workflow to achieve a DFTB parametrization was properly implemented.

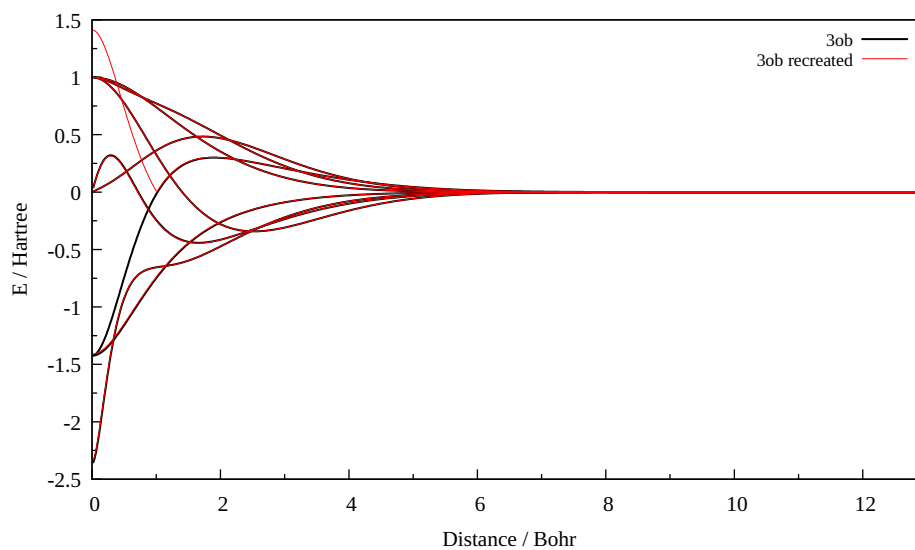


Figure S1: Comparison of the C-C Slater-Koster tables of original 3ob parametrization (black) and recreated one with Hotcent (red)

Table S1: Hubbard derivatives of Alkali metals from the original 3ob set^[2] and recalculated with Hotcent

Metal atom	3ob	Hotcent
Na	-0.0454	-0.0455
K	-0.0339	-0.0339

S2 Geometry optimisation benchmark of reference molecules

Table S2: Geometrical parameters of the molecular minimum structures

Molecule	MP2/cc-pVTZ	DFTB
Methylithium (d_{C-Li})	1.985	1.995
Coronene ($d_{plane-Li}$)	2.618	2.697

S3 Depiction of the scan configurations for the DFTB force field parametrisation

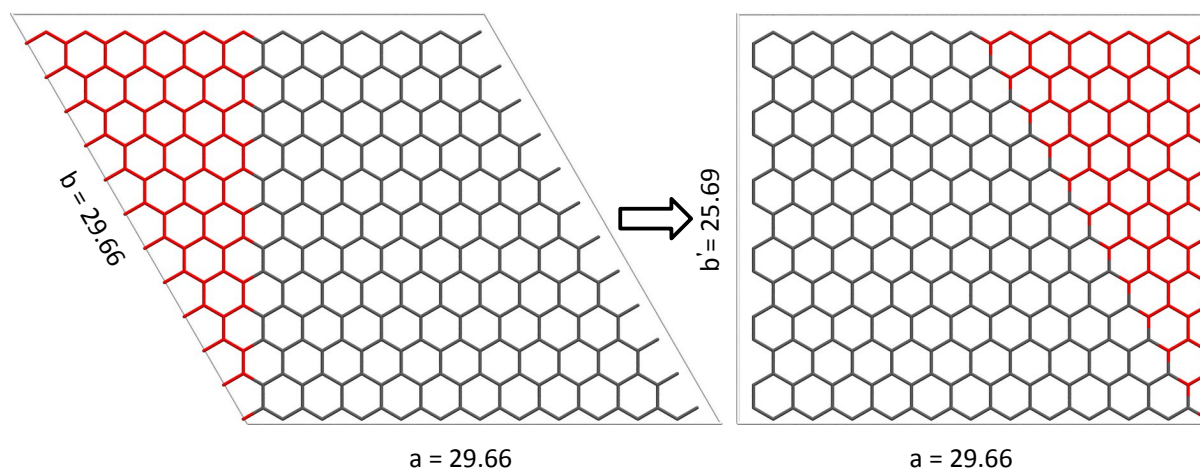


Figure S2: Orthorhombisation of the 12×12 graphene super cell, the carbon atoms coloured in red were shifted by a in x direction accordingly. The orthorhombisation is valid if the number of unit cells along the b -direction is even (twelve in this case).

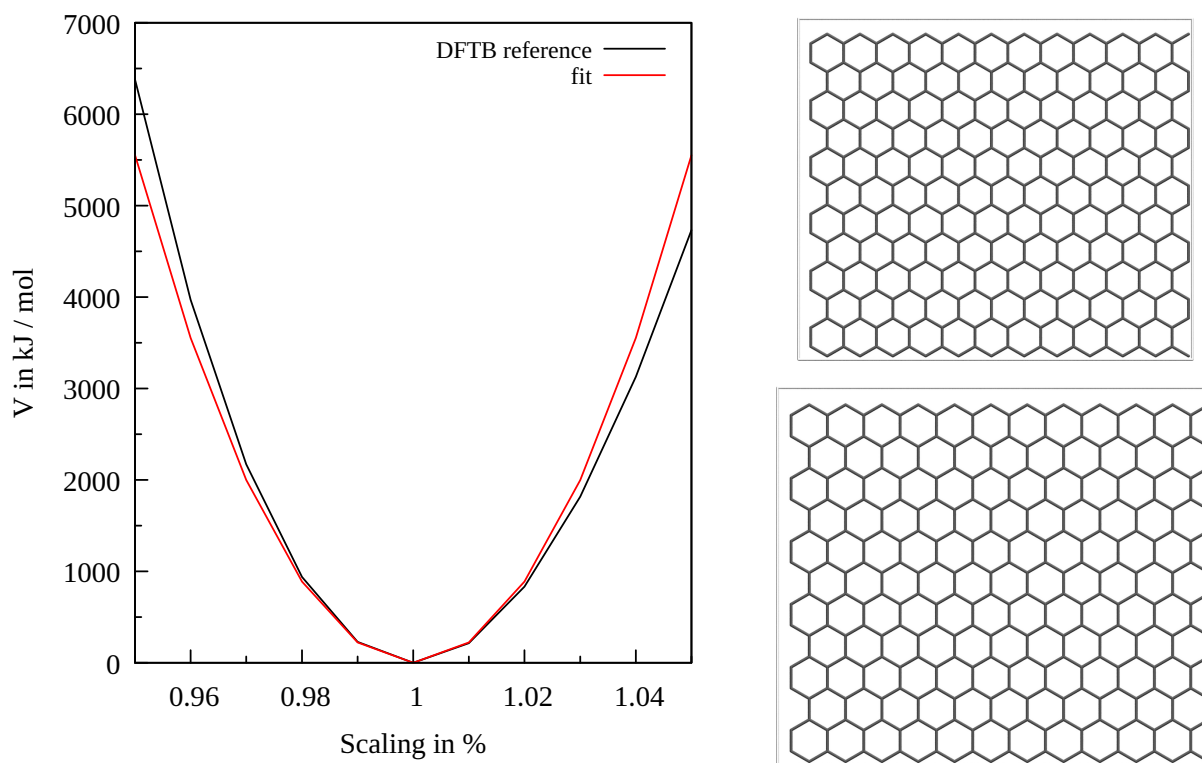


Figure S3: Visualisation of the bond potential of the force field and DFTB reference (left) and the associated scaled unit cell to 95% (upper right) and 105% (lower right)

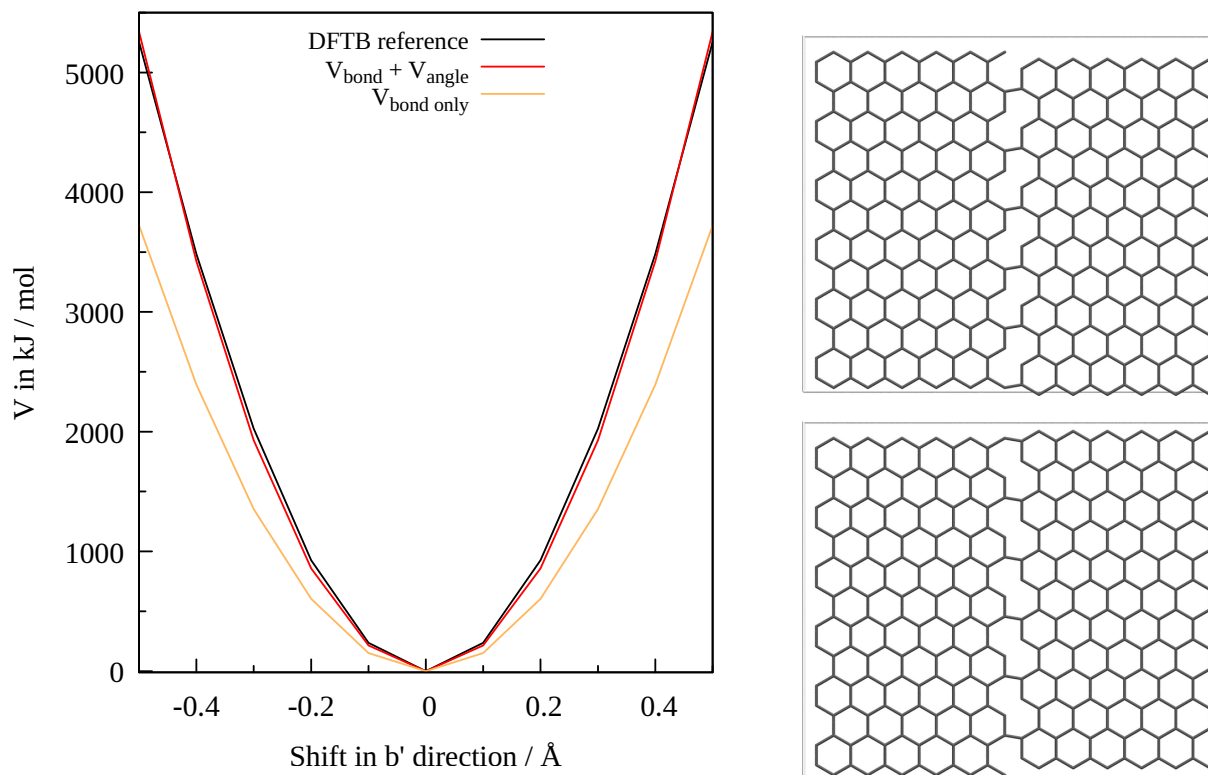


Figure S4: Visualisation of the angle potential of the force field and DFTB reference (left) and the associated shift of 0.5 and -0.5 Å in b' direction (right)

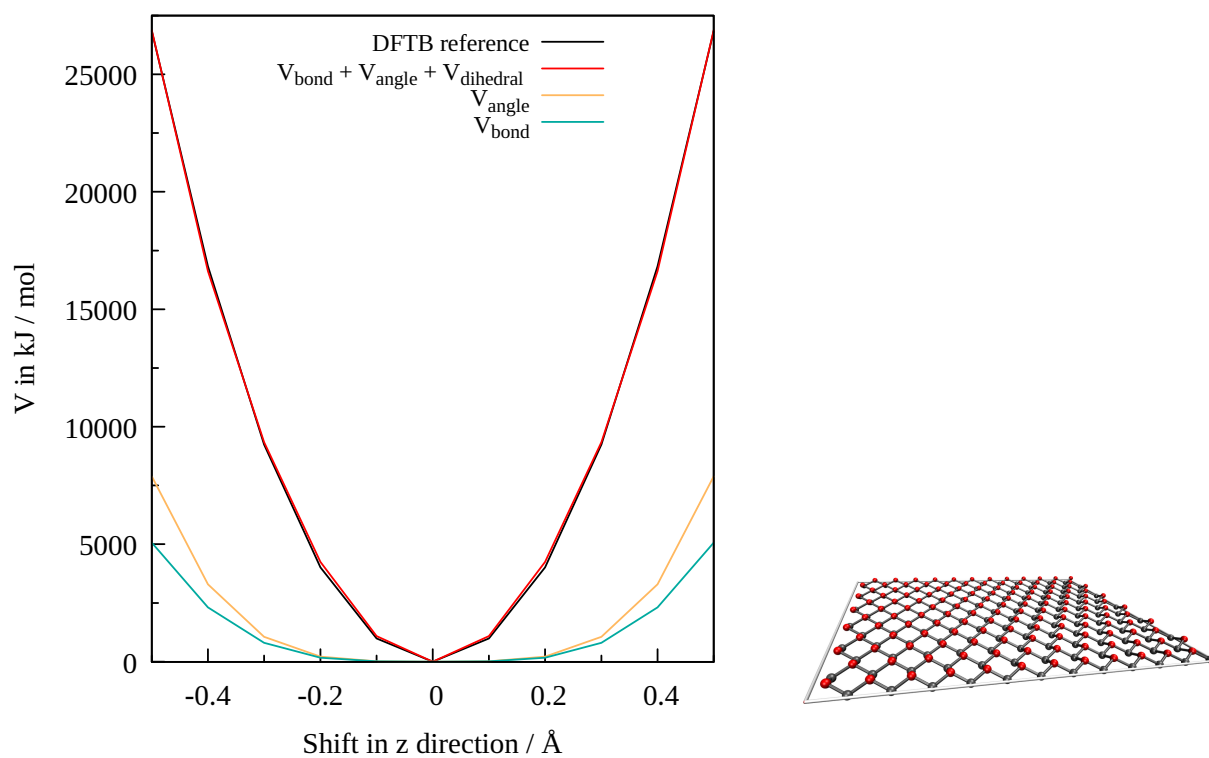


Figure S5: Visualisation of the dihedral potential of the force field and DFTB reference (left) and the associated shift of 0.5 and -0.5 Å in z direction (right)

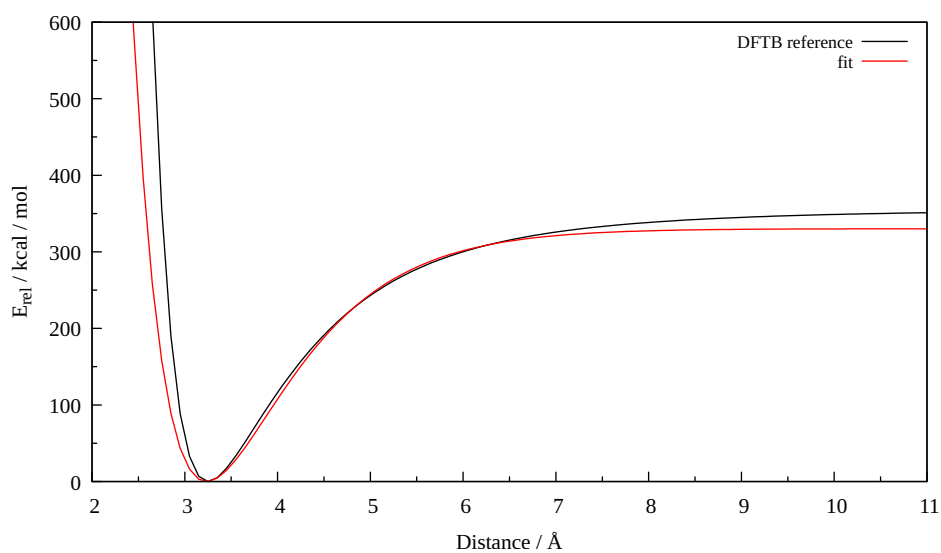


Figure S6: Energy plot of DFTB graphene interlayer scan and parametrised Morse potential

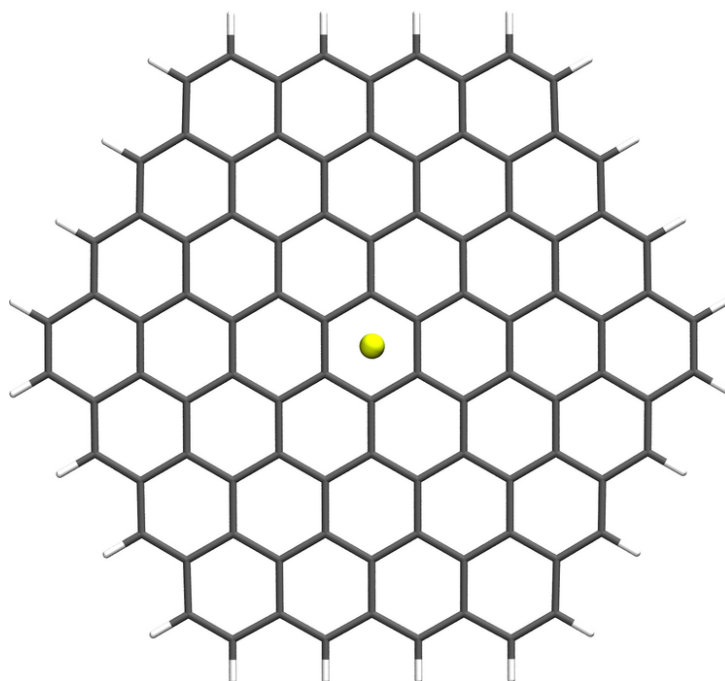


Figure S7: Visualisation of the graphene flake and adsorbed metal (Li/Na) atom employed in the scan with the composition $C_{96}H_{24}$

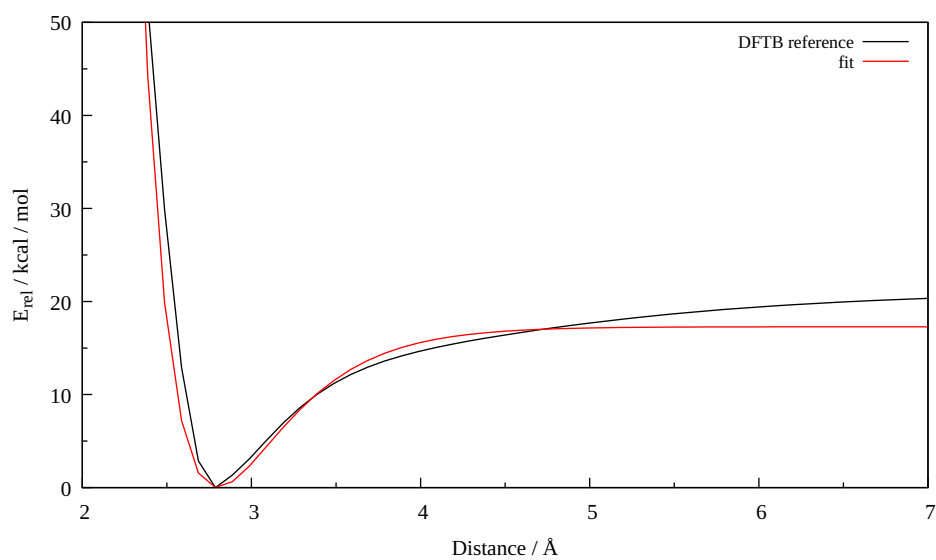


Figure S8: Energy plot of DFTB coronene and Li^0 scan and parametrised Morse potential

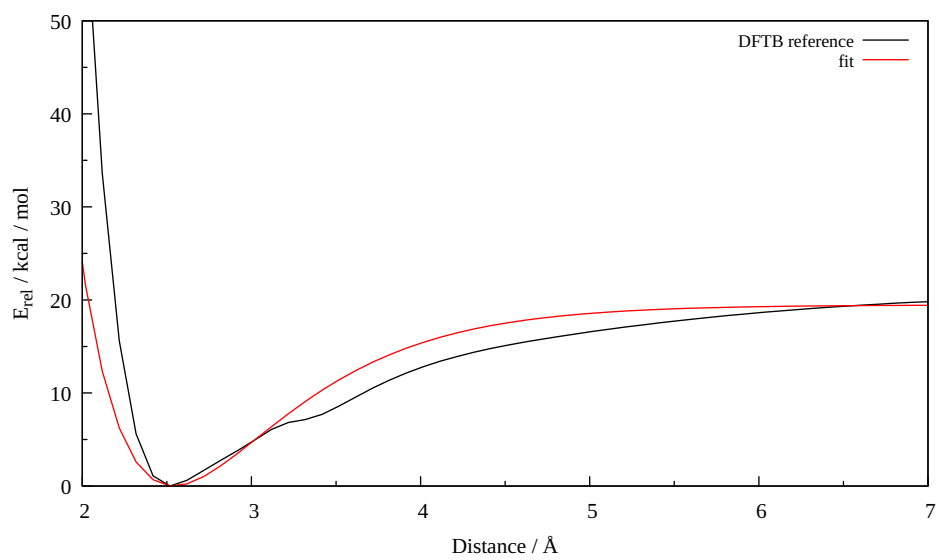


Figure S9: Energy plot of DFTB coronene and Na^0 scan and parametrised Morse potential

Table S3: Average charges of the alkali metal atoms in elementary charge e in dependence of the temperature over the simulation time

Metal	N_{Atoms}	Temperature / K	Charge / e
Li	1	273	0.5398
		298	0.5310
		323	0.5392
Li	2	273	0.5243
		298	0.5248
		323	0.5265
Li	4	273	0.5584
		298	0.5547
		323	0.5607
Na	1	273	0.6589
		298	0.6579
		323	0.6576
Na	2	273	0.6532
		298	0.6213
		323	0.6542
Na	4	273	0.6305
		298	0.6378
		323	0.6010

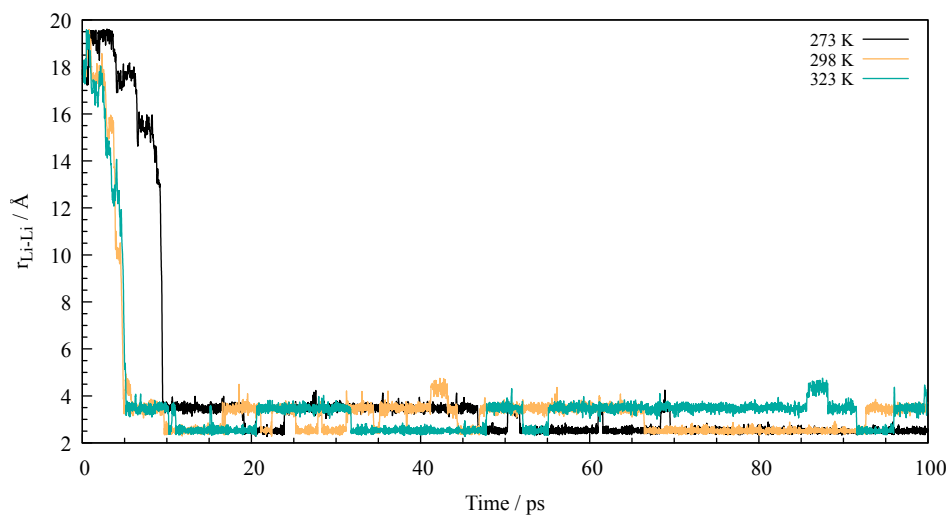


Figure S10: Distance between the two intercalated Li atoms at different temperatures (273 K, 298 K and 323 K) over the simulation time

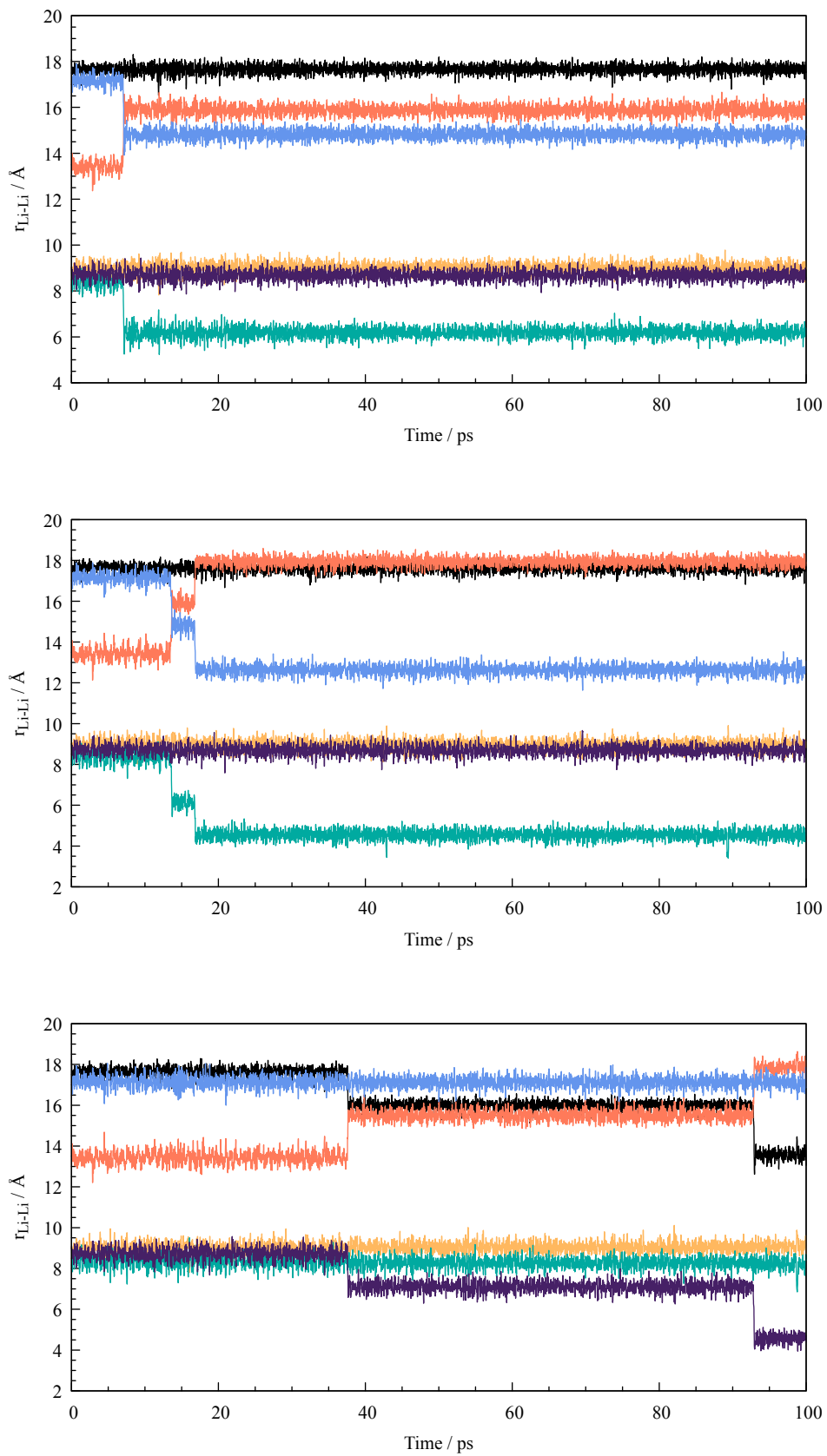


Figure S11: Distance between the Li atom pairs at 273 K (top), 298 K (center) and 323 K (bottom) of the simulations with four intercalated atoms

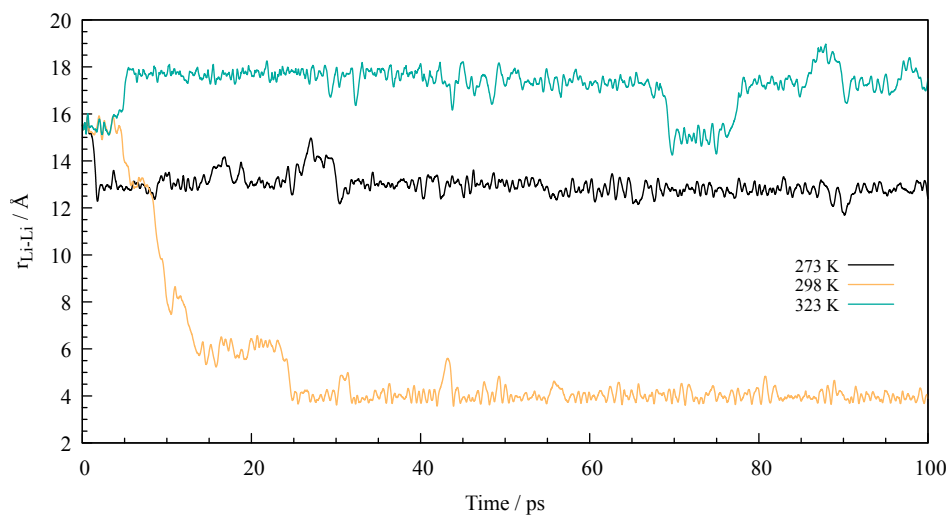


Figure S12: Distance between the two intercalated Na atoms at different temperatures (273 K, 298 K and 323 K) over the simulation time

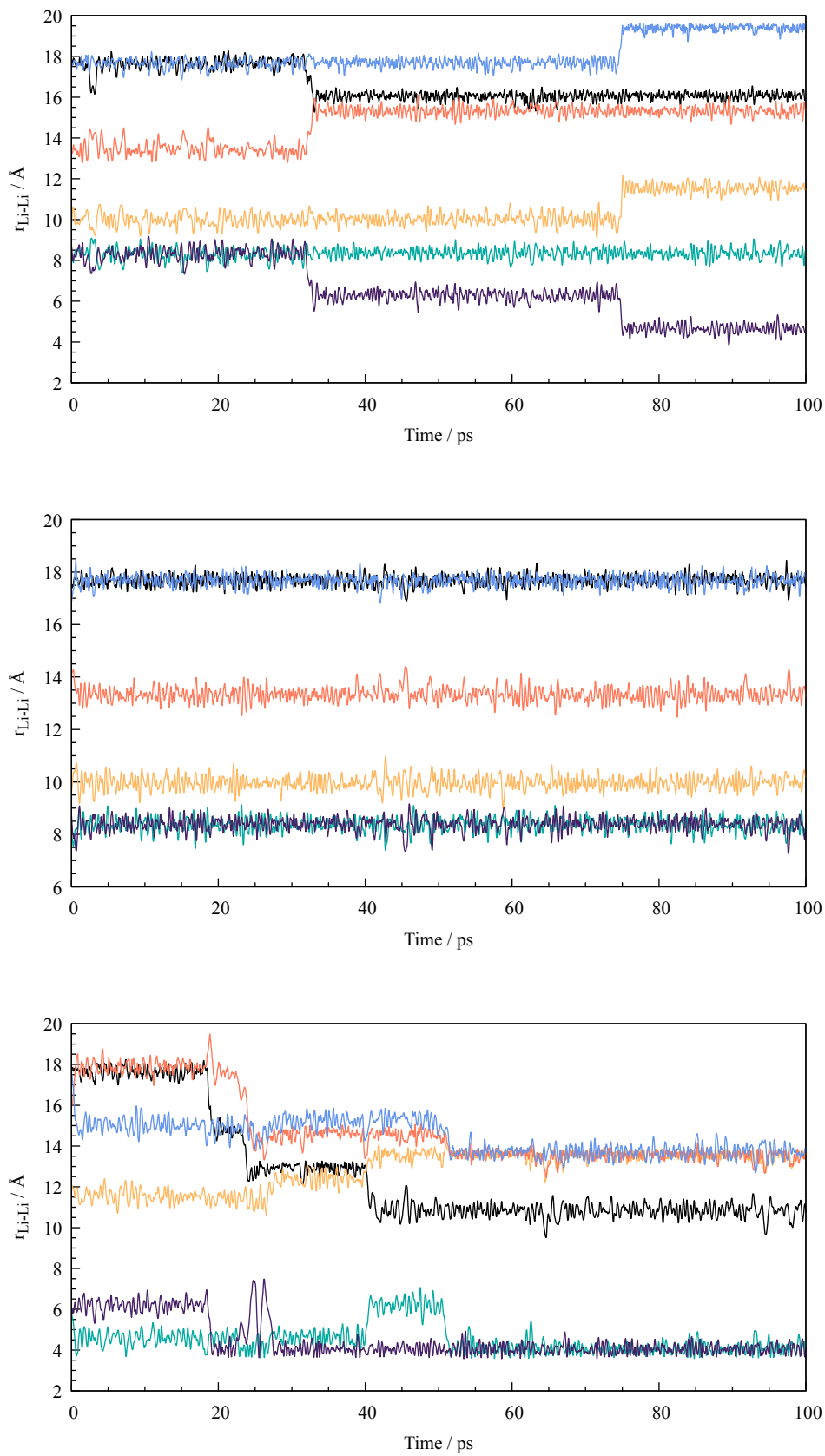


Figure S13: Distance between the Na atom pairs at 273 K (top), 298 K (center) and 323 K (bottom) of the simulations with four intercalated atoms

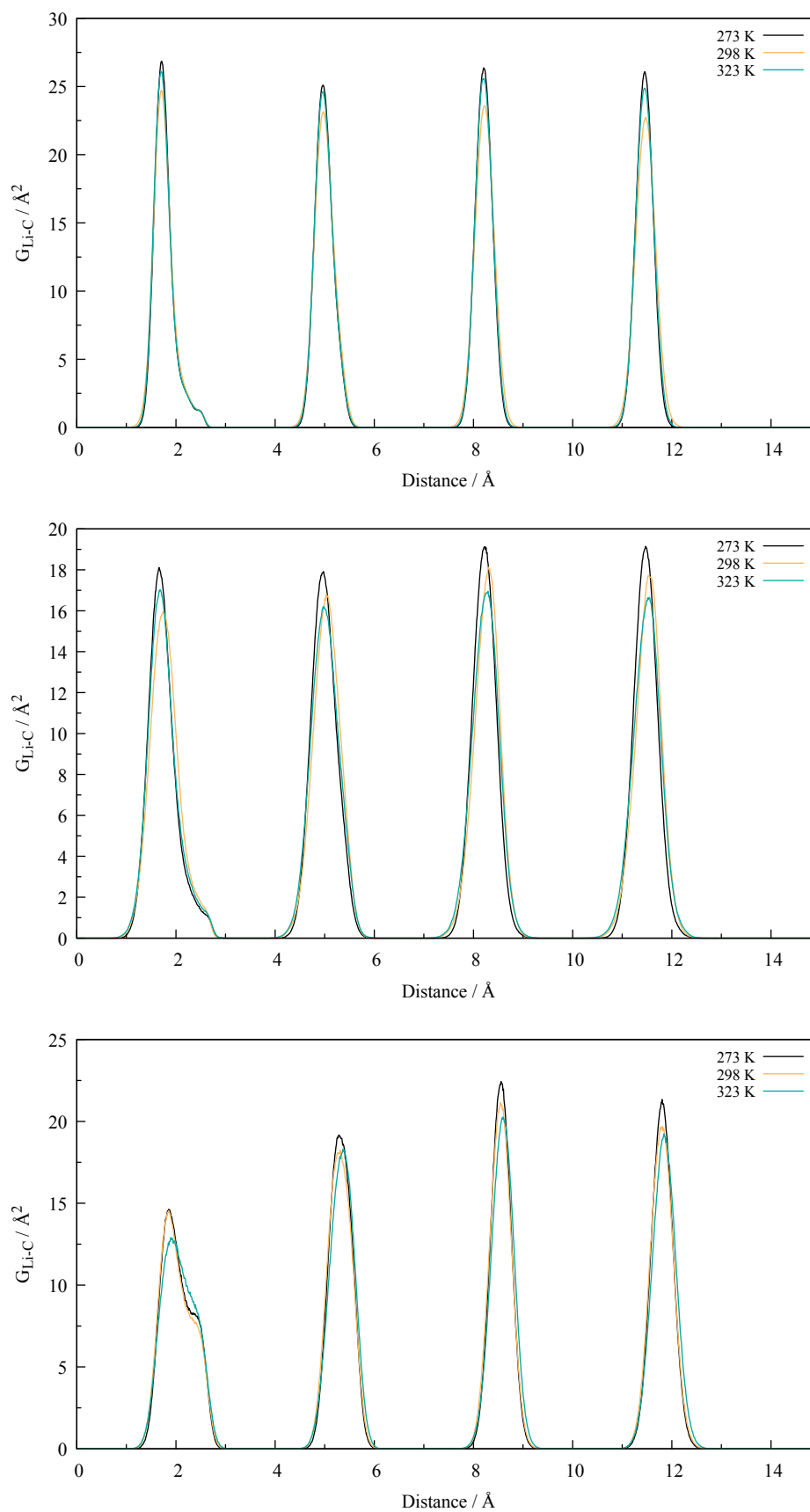


Figure S14: z-distribution functions of Li-C calculated from the simulation trajectories of the intercalation of one (top), two (center) and four (bottom) lithium atoms

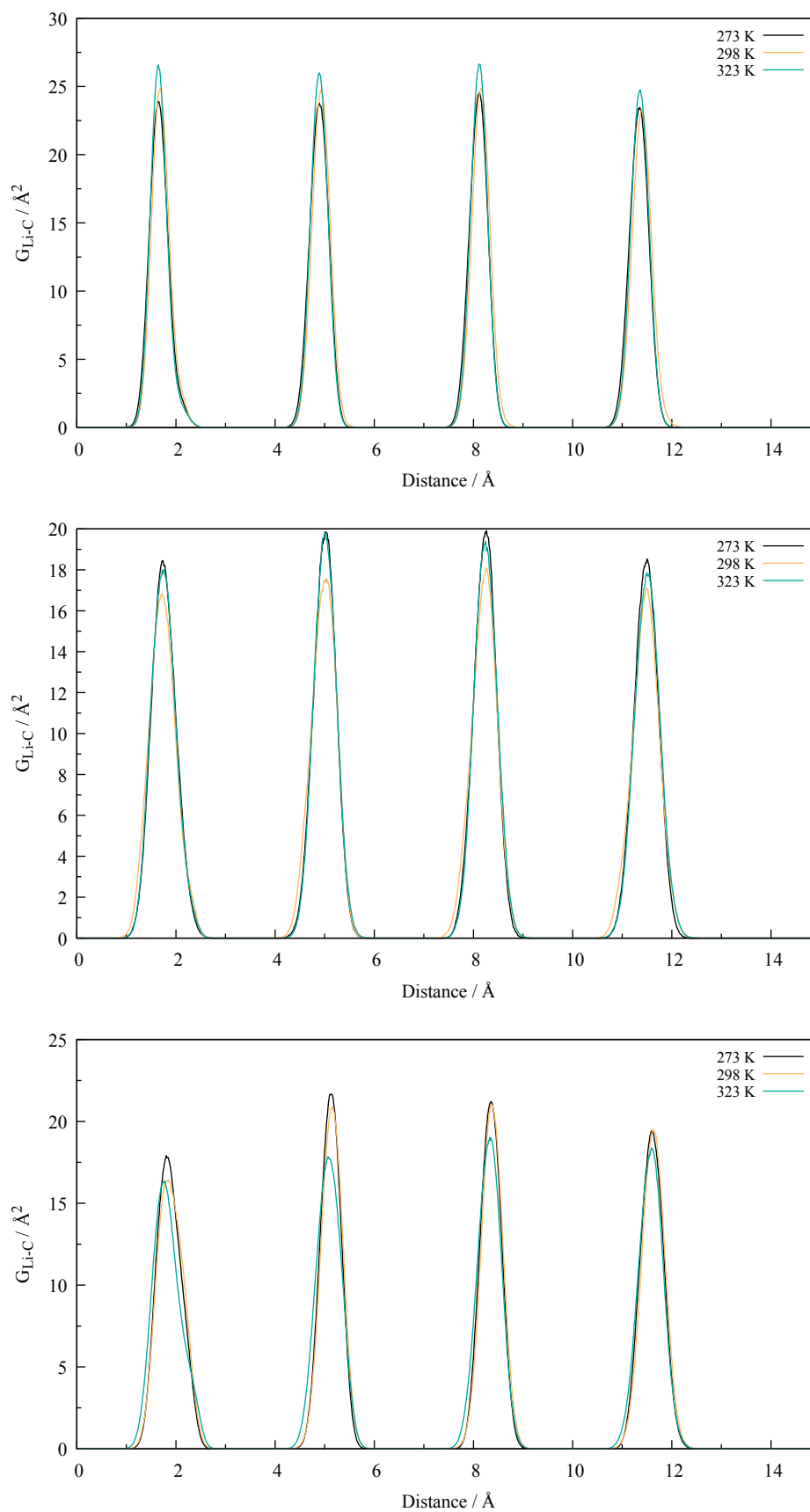


Figure S15: z -distribution functions of Na-C calculated from the simulation trajectories of the intercalation of one (top), two (center) and four (bottom) sodium atoms

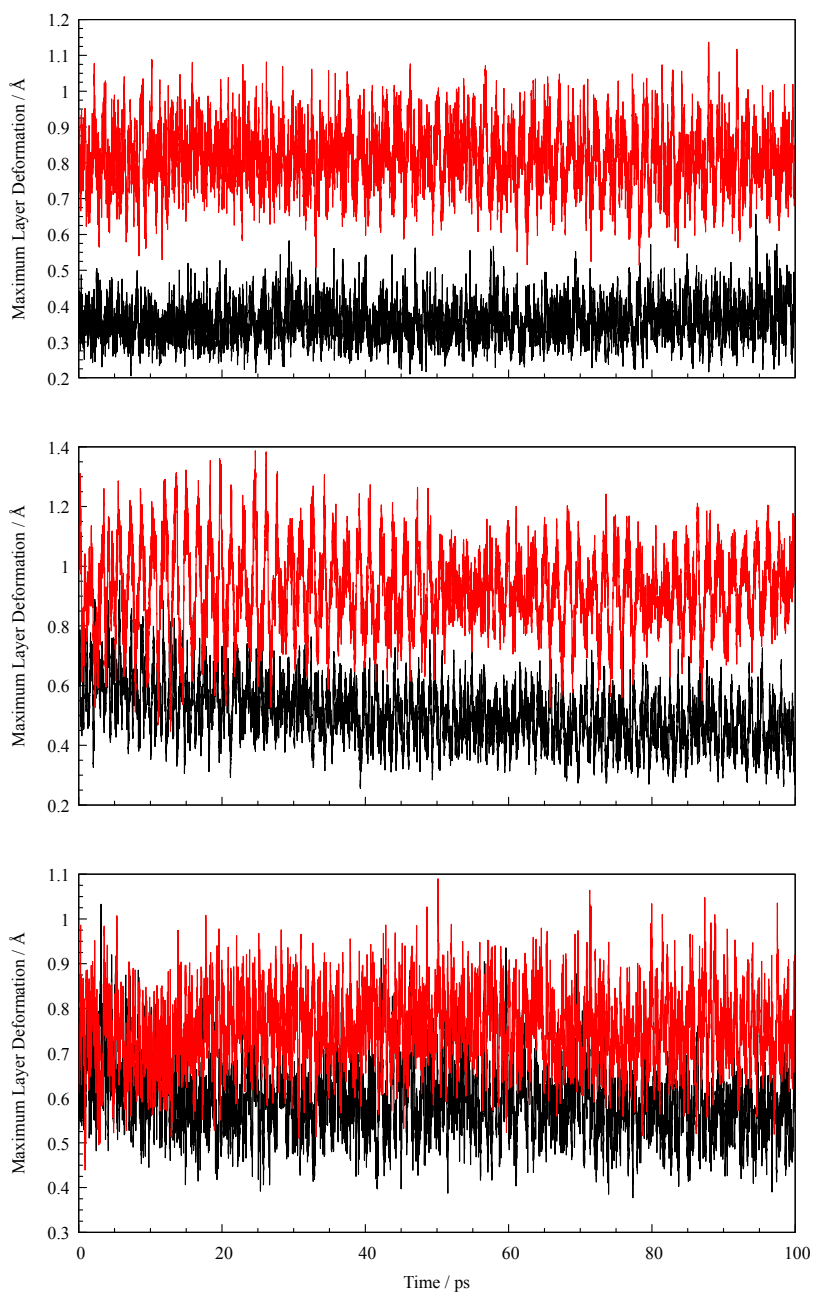


Figure S16: Maximum graphene plane deformations over time of the individual QM layers (black and red) intercalating one (top), two (center) and four (bottom) lithium atoms

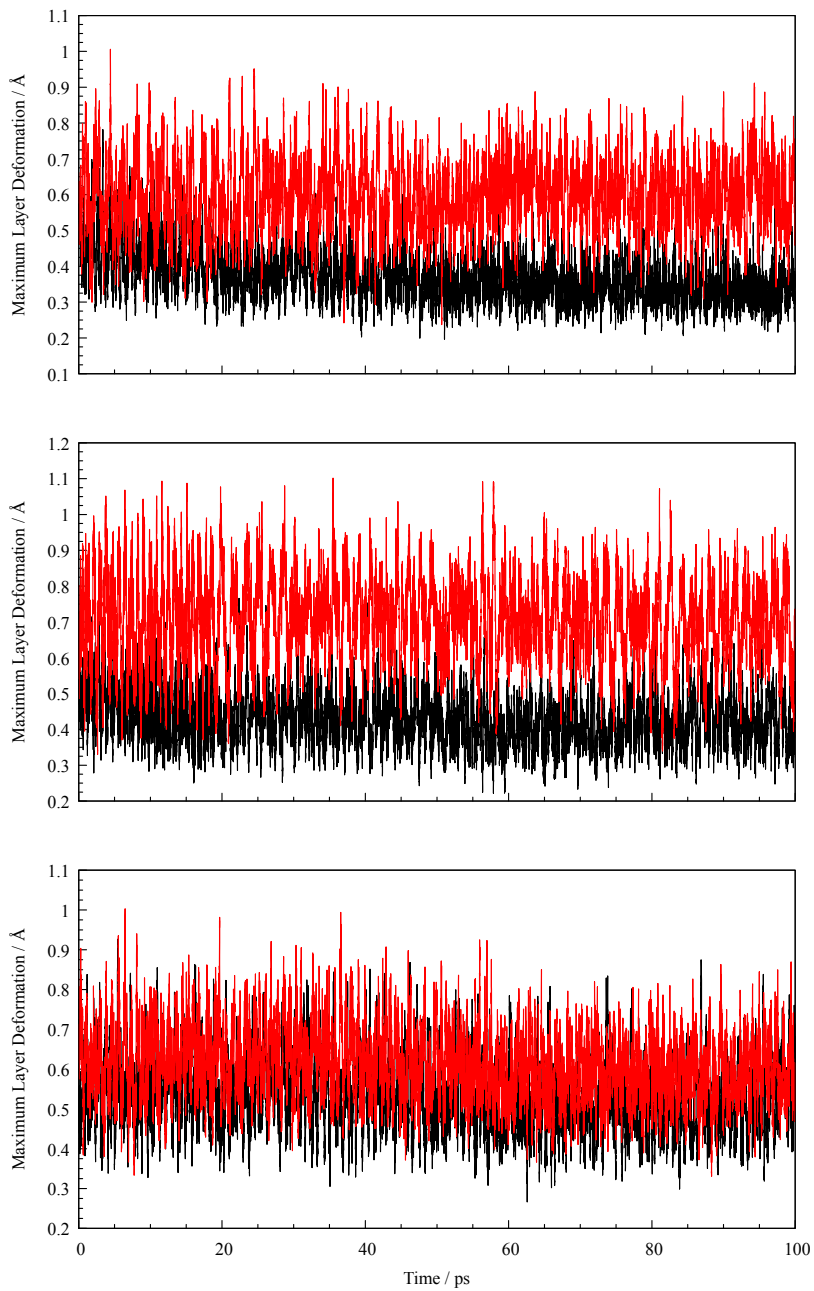


Figure S17: Maximum graphene plane deformations over time of the individual QM layers (black and red) intercalating one (top), two (center) and four (bottom) sodium atoms

Listing 1: MP2/cc-pVTZ optimised Methyllithium

5			
C	0.000000	0.000000	0.390478
Li	0.000000	0.000000	-1.594781
H	0.000000	1.009875	0.813825
H	-0.874578	-0.504938	0.813825
H	0.874578	-0.504938	0.813825

Listing 2: DFTB optimised Methyllithium

5			
C	-0.00000000	0.00001336	0.46522519
Li	0.00000000	-0.00000013	-1.52957324
H	0.00000000	1.03582104	0.76647492
H	-0.89705715	-0.51791663	0.76647856
H	0.89705715	-0.51791663	0.76647856

Listing 3: MP2 optimised Li in contact with coronene

37			
C	3.525541	1.240886	-0.044435
C	2.843516	-0.000412	-0.049309
C	3.525181	-1.241907	-0.044435
C	2.837520	-2.432554	-0.044200
C	1.421552	-2.462586	-0.052418
C	0.687195	-3.673615	-0.044352
C	2.838224	2.431732	-0.044200
C	1.422265	2.462174	-0.052418
C	0.710937	1.230479	-0.057826
C	1.421283	-0.000206	-0.066198
C	0.710581	-1.230684	-0.057826
C	-0.710419	-1.230552	-0.066506
C	-1.421749	-2.462159	-0.049725
C	-0.687768	-3.673455	-0.044763

C	0.688259	3.673416	-0.044352
C	-0.686704	3.673654	-0.044763
C	-1.421036	2.462571	-0.049725
C	-0.710063	1.230758	-0.066506
C	-1.420737	0.000206	-0.058193
C	-2.843111	0.000412	-0.053063
C	-3.525060	-1.240881	-0.045038
C	-2.837747	-2.431735	-0.045146
C	-2.837043	2.432556	-0.045146
C	-3.524701	1.241902	-0.045038
H	4.608396	-1.240707	-0.033292
H	3.377850	-3.371422	-0.036566
H	4.608755	1.239373	-0.033292
H	1.229843	-4.611146	-0.036675
H	3.378826	3.370444	-0.036566
H	-1.230684	-4.610789	-0.033690
H	1.231178	4.610790	-0.036675
H	-3.378316	-3.370426	-0.034079
H	-1.229349	4.611145	-0.033690
H	-3.377340	3.371404	-0.034079
H	-4.607950	1.240737	-0.037615
H	-4.608309	-1.239402	-0.037615
Li	-0.012795	0.000002	2.572445

Listing 4: DFTB optimised Li in contact with coronene

37

C	-3.68624267	-0.68967426	0.06740591
C	-3.68652238	0.68911036	0.06162971
C	-1.24118305	-3.54511156	0.08454014
C	-2.43530343	-2.85587827	0.07843183
C	-2.46641304	-1.42951225	0.07034154
C	-1.23177782	-0.71646815	0.06745921
C	-1.23198051	0.71662313	0.06156515
C	-2.46682478	1.42935164	0.05884120

C	-2.43593361	2.85569231	0.05620321
C	-1.24186421	3.54521711	0.05613742
C	1.26024894	-3.54476135	0.09061372
C	0.00955462	-2.85855344	0.08235733
C	0.00940856	-1.43284282	0.07354166
C	1.25046775	-0.71618149	0.07373154
C	1.25026998	0.71692130	0.06776605
C	0.00907304	1.43333439	0.06166346
C	0.00894492	2.85909265	0.05884477
C	1.25974661	3.54560420	0.06146921
C	2.45434438	-2.85524058	0.09081310
C	2.48519335	-1.42893337	0.08264030
C	3.70495218	-0.68880160	0.08509471
C	3.70475548	0.69002234	0.07895659
C	2.48496870	1.42988136	0.07066501
C	2.45381567	2.85629533	0.06745710
H	-3.37721852	-3.40057054	0.07823304
H	-4.62876919	-1.23327476	0.06877598
H	-4.62931705	1.23222594	0.05776767
H	-3.37782405	3.40039278	0.05306136
H	-1.24172699	-4.63317750	0.08992593
H	-1.24279068	4.63326274	0.05293052
H	1.26090193	-4.63282265	0.09532466
H	1.26043800	4.63368302	0.05733461
H	3.39629499	-3.39980648	0.09567538
H	4.64764795	-1.23208425	0.09054409
H	4.64731840	1.23357738	0.07882272
H	3.39570160	3.40106528	0.06866506
Li	0.00249405	0.01146193	2.76925922

Listing 5: DFTB optimised Li in contact with a graphene flake with composition $C_{96}H_{24}$

121

C	-3.73656159	-0.60807528	0.22260823	4.00723830
C	-3.74100305	0.81712682	0.20999253	4.00724321

C	-1.25561024	-3.45733218	0.21820375	4.00723980
C	-2.49204919	-2.74842842	0.22642565	4.00723264
C	-2.50052739	-1.32137974	0.22204905	4.01367433
C	-1.26737034	-0.60441110	0.20564162	4.01570273
C	-1.27184253	0.82848681	0.19256445	4.01570735
C	-2.50943372	1.53797208	0.19654057	4.01368327
C	-2.50982916	2.96490018	0.17567570	4.00725016
C	-1.27782470	3.68118428	0.15354696	4.00725506
C	1.22008487	-3.44992606	0.18905763	4.00725217
C	-0.01987430	-2.74365086	0.20511678	4.01367748
C	-0.02425450	-1.31715109	0.19687557	4.01570063
C	1.21440638	-0.59700193	0.17455351	4.01569999
C	1.20992201	0.83588834	0.16065765	4.01569756
C	-0.03318606	1.54863320	0.16996144	4.01569939
C	-0.03769009	2.97504085	0.15169220	4.01367834
C	1.19782145	3.68855490	0.12064341	4.00724563
C	2.45209728	-2.73364152	0.16741597	4.00725623
C	2.45188121	-1.30657609	0.16116576	4.01368932
C	3.68323048	-0.58589341	0.13030298	4.00724760
C	3.67875502	0.83928581	0.11547424	4.00723573
C	2.44292737	1.55274445	0.13241185	4.01366903
C	2.43423568	2.97963147	0.11069045	4.00723498
Li	0.00490745	0.14076015	2.83578697	0.48421568
C	4.91372007	1.55912895	0.07544552	4.00109546
C	3.67083376	3.69668911	0.07109093	4.00109669
C	1.19155524	5.11824657	0.09149538	4.00109961
C	-1.28085839	5.11089132	0.12450415	4.00110334
C	-3.75129876	3.67456327	0.16796160	4.00110101
C	-4.98086869	1.52957792	0.20147943	4.00109772
C	-4.97197370	-1.32825443	0.22720207	4.00109884
C	-3.72908465	-3.46581455	0.23080065	4.00109479
C	-1.24974821	-4.88731850	0.21474071	4.00109776
C	1.22271953	-4.87992468	0.18604947	4.00110133
C	3.69317721	-3.44361085	0.14301135	4.00110535
C	4.90647555	2.98499226	0.05315641	3.99788115

C	2.42572310	5.83046514	0.05269431	3.99890912
C	3.66162078	5.12182519	0.04236791	3.99890307
C	-0.04695559	5.82516291	0.09378419	3.99788854
C	-2.51984280	5.81574407	0.11818831	3.99891150
C	-3.75134551	5.09973521	0.13938457	3.99890506
C	-4.98272329	2.95547797	0.18034621	3.99788346
C	-6.21084990	0.80911663	0.20577754	3.99890345
C	-6.20641318	-0.61549253	0.21899064	3.99890470
C	-4.96495274	-2.75428723	0.23123009	3.99788305
C	-3.72026907	-4.89123700	0.22679595	3.99889970
C	-2.48433911	-5.59984772	0.21904171	3.99890537
C	-0.01140540	-5.59435508	0.19890133	3.99788625
C	2.46132053	-5.58505638	0.16157843	3.99890863
C	3.69283178	-4.86906639	0.14026702	3.99890526
C	4.92270333	-1.29865965	0.10589476	4.00110404
C	4.92439451	-2.72470003	0.11271912	3.99789134
C	6.14775580	0.84605303	0.05063395	3.99890375
C	6.15224897	-0.57853345	0.06625271	3.99890669
C	4.90765437	5.83539839	-0.00291170	3.95137636
C	2.41161251	7.26657952	0.01792955	3.95137031
C	-0.05170679	7.26048524	0.05791153	3.94949649
C	-2.51521280	7.25191675	0.08317627	3.95137200
C	-5.00236952	5.80583437	0.12504801	3.95137649
C	-6.22839136	3.66927244	0.16377258	3.94949932
C	-7.45255058	1.53144479	0.18936477	3.95137071
C	-7.44360427	-1.34570130	0.21713435	3.95137374
C	-6.20616242	-3.47599053	0.22858350	3.94950174
C	-4.96688006	-5.60523579	0.22436251	3.95137394
C	-2.47077764	-7.03635471	0.20924729	3.95136967
C	-0.00722802	-7.03009006	0.18869100	3.94949757
C	2.45612219	-7.02161755	0.15151253	3.95137192
C	4.94329488	-5.57559442	0.10856202	3.95137362
C	6.16950889	-3.43896309	0.08130512	3.94950176
C	7.39341463	-1.30132017	0.03568917	3.95137163
C	7.38432392	1.57579427	0.00348027	3.95137269

C	6.14706756	3.70623302	0.00618273	3.94950053
C	3.67794915	7.95602139	-0.02365937	4.10700600
C	4.86251171	7.27681939	-0.03347391	4.10700301
C	1.18963764	7.94933291	0.02210670	4.15259211
C	-1.29763877	7.94193711	0.05533847	4.15259237
C	-6.20457513	5.08894858	0.13787868	4.15257606
C	-7.42387641	-2.74532443	0.22352678	4.15257722
C	-6.17351672	-4.89572360	0.22644106	4.15257504
C	-1.24892047	-7.71919675	0.19599938	4.15258932
C	1.23839211	-7.71175452	0.16665320	4.15258695
C	3.72669926	-7.70381936	0.12144779	4.10700016
C	4.90705469	-7.01757193	0.10109973	4.10700227
C	6.14536918	-4.85887041	0.08179864	4.15258562
C	7.38231014	-2.70102281	0.04537406	4.15258723
C	8.61469884	0.82341214	-0.02442221	4.10699702
C	8.61902680	-0.54199233	-0.00869987	4.10700415
C	7.36441014	2.97528541	-0.01683170	4.15257378
C	6.11409863	5.12573683	-0.01924714	4.15257862
C	-4.96664254	7.24750167	0.09366020	4.10700232
C	-3.78629366	7.93378654	0.07409077	4.10700672
C	-7.44152994	2.93104019	0.16967670	4.15257323
C	-8.67871137	0.77170513	0.19031902	4.10699802
C	-8.67446745	-0.59371698	0.20404277	4.10700003
C	-4.92219555	-7.04697209	0.21650259	4.10699767
C	-3.73760426	-7.72614945	0.20963575	4.10700278
H	1.18719919	9.03757550	-0.00861194	0.91732887
H	-1.30249814	9.03017484	0.02472794	0.91732896
H	-3.78887923	9.02186298	0.04803185	0.91906489
H	-5.91142587	7.78775254	0.08315882	0.91906472
H	-7.14848334	5.63117020	0.12183464	0.91732819
H	-8.38663295	3.47114525	0.15264150	0.91732788
H	-9.62247887	1.31367202	0.17717976	0.91906304
H	-9.61485102	-1.14168867	0.20208597	0.91906425
H	-8.36561535	-3.29151505	0.21825667	0.91733025
H	-7.11404110	-5.44399491	0.22049218	0.91732967

H	-5.86360604	-7.59317132	0.21372582	0.91906426
H	-3.73341678	-8.81450157	0.20152178	0.91906440
H	-1.24699821	-8.80781704	0.18491871	0.91732963
H	1.24271760	-8.80036255	0.15504752	0.91732921
H	3.72880782	-8.79216839	0.11204088	0.91906307
H	5.85137189	-7.55812949	0.07541258	0.91906310
H	7.08876270	-5.40151194	0.05398231	0.91732879
H	8.32692383	-3.24157081	0.01820423	0.91732920
H	9.56237241	-1.08431738	-0.03277101	0.91906390
H	9.55459107	1.37099847	-0.06113896	0.91906320
H	8.30557801	3.52104106	-0.05656456	0.91732917
H	7.05407889	5.67362264	-0.05773881	0.91733005
H	5.80348536	7.82272452	-0.06737917	0.91906537
H	3.67336017	9.04408593	-0.04986287	0.91906504

Listing 6: DFTB optimised dual layer graphene

576				
C	2.31257874	0.26404189	2.34557151	4.00116479
C	1.07700354	0.97740413	2.34646095	3.99883517
C	1.07700355	2.40409541	2.34557862	4.00116483
C	2.31257875	3.11745768	2.34646342	3.99883515
C	2.31257876	4.54414900	2.34557654	4.00116483
C	1.07700355	5.25751127	2.34646271	3.99883519
C	1.07700354	6.68420260	2.34557852	4.00116480
C	2.31257874	7.39756485	2.34646498	3.99883525
C	2.31257870	8.82425614	2.34558308	4.00116477
C	1.07700350	9.53761840	2.34647059	3.99883525
C	1.07700349	10.96430968	2.34558442	4.00116477
C	2.31257869	11.67767191	2.34646823	3.99883524
C	2.31257871	13.10436317	2.34558053	4.00116480
C	1.07700353	13.81772546	2.34646624	3.99883519
C	1.07700358	15.24441676	2.34557899	4.00116483
C	2.31257878	15.95777905	2.34646285	3.99883517
C	2.31257883	17.38447039	2.34557676	4.00116483

C	1.07700366	18.09783271	2.34646369	3.99883517
C	1.07700368	19.52452405	2.34557778	4.00116481
C	2.31257885	20.23788635	2.34646142	3.99883522
C	2.31257883	21.66457767	2.34557132	4.00116477
C	1.07700364	22.37793993	2.34645510	3.99883526
C	1.07700362	23.80463120	2.34556690	4.00116476
C	2.31257879	24.51799345	2.34645228	3.99883525
C	4.78372908	0.26404183	2.34557364	4.00116479
C	3.54815393	0.97740412	2.34646037	3.99883518
C	3.54815393	2.40409540	2.34557786	4.00116483
C	4.78372913	3.11745762	2.34646544	3.99883514
C	4.78372913	4.54414894	2.34557865	4.00116483
C	3.54815396	5.25751125	2.34646212	3.99883520
C	3.54815393	6.68420257	2.34557780	4.00116479
C	4.78372912	7.39756479	2.34646698	3.99883524
C	4.78372907	8.82425609	2.34558511	4.00116477
C	3.54815390	9.53761837	2.34647022	3.99883526
C	3.54815387	10.96430964	2.34558409	4.00116477
C	4.78372905	11.67767186	2.34647029	3.99883523
C	4.78372905	13.10436312	2.34558263	4.00116480
C	3.54815390	13.81772542	2.34646570	3.99883520
C	3.54815394	15.24441672	2.34557822	4.00116483
C	4.78372911	15.95777900	2.34646498	3.99883516
C	4.78372915	17.38447033	2.34557895	4.00116484
C	3.54815401	18.09783268	2.34646321	3.99883517
C	3.54815401	19.52452403	2.34557733	4.00116481
C	4.78372917	20.23788630	2.34646350	3.99883520
C	4.78372914	21.66457761	2.34557340	4.00116477
C	3.54815400	22.37793992	2.34645476	3.99883526
C	3.54815397	23.80463119	2.34556650	4.00116476
C	4.78372914	24.51799339	2.34645440	3.99883524
C	7.25487938	0.26404169	2.34557561	4.00116480
C	6.01930426	0.97740402	2.34646369	3.99883515
C	6.01930427	2.40409529	2.34558126	4.00116484
C	7.25487943	3.11745751	2.34646770	3.99883512

C	7.25487943	4.54414882	2.34558076	4.00116484
C	6.01930430	5.25751117	2.34646551	3.99883517
C	6.01930427	6.68420248	2.34558118	4.00116480
C	7.25487942	7.39756473	2.34646919	3.99883522
C	7.25487938	8.82425603	2.34558693	4.00116478
C	6.01930424	9.53761832	2.34647329	3.99883523
C	6.01930420	10.96430958	2.34558713	4.00116478
C	7.25487934	11.67767183	2.34647201	3.99883521
C	7.25487934	13.10436309	2.34558450	4.00116481
C	6.01930421	13.81772538	2.34646900	3.99883517
C	6.01930424	15.24441667	2.34558174	4.00116484
C	7.25487939	15.95777897	2.34646745	3.99883514
C	7.25487943	17.38447028	2.34558109	4.00116485
C	6.01930430	18.09783262	2.34646657	3.99883515
C	6.01930430	19.52452396	2.34558053	4.00116482
C	7.25487945	20.23788622	2.34646526	3.99883519
C	7.25487943	21.66457751	2.34557501	4.00116478
C	6.01930430	22.37793983	2.34645782	3.99883524
C	6.01930427	23.80463108	2.34556964	4.00116476
C	7.25487943	24.51799327	2.34645631	3.99883522
C	9.72602963	0.26404160	2.34557325	4.00116479
C	8.49045453	0.97740390	2.34646306	3.99883516
C	8.49045454	2.40409517	2.34558083	4.00116483
C	9.72602966	3.11745744	2.34646546	3.99883514
C	9.72602967	4.54414875	2.34557849	4.00116483
C	8.49045456	5.25751109	2.34646497	3.99883518
C	8.49045454	6.68420241	2.34558084	4.00116480
C	9.72602964	7.39756471	2.34646703	3.99883524
C	9.72602960	8.82425601	2.34558448	4.00116477
C	8.49045449	9.53761829	2.34647231	3.99883524
C	8.49045446	10.96430956	2.34558615	4.00116478
C	9.72602956	11.67767185	2.34646945	3.99883523
C	9.72602958	13.10436310	2.34558209	4.00116480
C	8.49045447	13.81772538	2.34646842	3.99883518
C	8.49045451	15.24441666	2.34558157	4.00116483

C	9.72602963	15.95777897	2.34646548	3.99883516
C	9.72602968	17.38447027	2.34557887	4.00116484
C	8.49045456	18.09783258	2.34646582	3.99883515
C	8.49045457	19.52452390	2.34557962	4.00116481
C	9.72602971	20.23788617	2.34646262	3.99883521
C	9.72602969	21.66457745	2.34557230	4.00116477
C	8.49045457	22.37793973	2.34645678	3.99883524
C	8.49045455	23.80463097	2.34556888	4.00116476
C	9.72602968	24.51799318	2.34645397	3.99883524
C	12.19717987	0.26404163	2.34557406	4.00116479
C	10.96160475	0.97740387	2.34646153	3.99883517
C	10.96160476	2.40409514	2.34557932	4.00116483
C	12.19717986	3.11745747	2.34646617	3.99883514
C	12.19717987	4.54414878	2.34557928	4.00116483
C	10.96160476	5.25751108	2.34646353	3.99883519
C	10.96160474	6.68420240	2.34557939	4.00116479
C	12.19717983	7.39756474	2.34646764	3.99883524
C	12.19717980	8.82425604	2.34558520	4.00116477
C	10.96160469	9.53761831	2.34647069	3.99883525
C	10.96160467	10.96430958	2.34558452	4.00116477
C	12.19717978	11.67767188	2.34647024	3.99883523
C	12.19717980	13.10436314	2.34558282	4.00116480
C	10.96160469	13.81772541	2.34646690	3.99883519
C	10.96160475	15.24441668	2.34558018	4.00116483
C	12.19717988	15.95777900	2.34646612	3.99883516
C	12.19717994	17.38447031	2.34557970	4.00116484
C	10.96160482	18.09783258	2.34646438	3.99883517
C	10.96160484	19.52452389	2.34557806	4.00116481
C	12.19717997	20.23788620	2.34646348	3.99883521
C	12.19717996	21.66457748	2.34557311	4.00116477
C	10.96160482	22.37793970	2.34645510	3.99883526
C	10.96160480	23.80463094	2.34556737	4.00116476
C	12.19717992	24.51799321	2.34645481	3.99883524
C	14.66833012	0.26404177	2.34557455	4.00116480
C	13.43275498	0.97740395	2.34646336	3.99883516

C	13.43275499	2.40409522	2.34558099	4.00116484
C	14.66833010	3.11745758	2.34646649	3.99883513
C	14.66833010	4.54414889	2.34557960	4.00116483
C	13.43275497	5.25751114	2.34646525	3.99883517
C	13.43275495	6.68420247	2.34558093	4.00116480
C	14.66833005	7.39756480	2.34646788	3.99883523
C	14.66833003	8.82425610	2.34558578	4.00116477
C	13.43275490	9.53761836	2.34647266	3.99883524
C	13.43275489	10.96430962	2.34558654	4.00116477
C	14.66833001	11.67767191	2.34647098	3.99883522
C	14.66833004	13.10436316	2.34558334	4.00116480
C	13.43275493	13.81772544	2.34646859	3.99883518
C	13.43275500	15.24441672	2.34558162	4.00116483
C	14.66833013	15.95777904	2.34646610	3.99883515
C	14.66833020	17.38447036	2.34557994	4.00116484
C	13.43275508	18.09783264	2.34646630	3.99883515
C	13.43275511	19.52452395	2.34558009	4.00116481
C	14.66833023	20.23788629	2.34646419	3.99883520
C	14.66833022	21.66457758	2.34557393	4.00116477
C	13.43275508	22.37793978	2.34645717	3.99883524
C	13.43275506	23.80463103	2.34556930	4.00116476
C	14.66833017	24.51799334	2.34645530	3.99883523
C	17.13948037	0.26404189	2.34557238	4.00116479
C	15.90390523	0.97740410	2.34646172	3.99883517
C	15.90390524	2.40409537	2.34557935	4.00116483
C	17.13948036	3.11745769	2.34646446	3.99883515
C	17.13948037	4.54414900	2.34557747	4.00116483
C	15.90390521	5.25751124	2.34646343	3.99883518
C	15.90390520	6.68420255	2.34557912	4.00116480
C	17.13948032	7.39756485	2.34646585	3.99883524
C	17.13948029	8.82425614	2.34558395	4.00116476
C	15.90390514	9.53761839	2.34647134	3.99883525
C	15.90390513	10.96430965	2.34558524	4.00116477
C	17.13948026	11.67767191	2.34646909	3.99883524
C	17.13948029	13.10436317	2.34558134	4.00116479

C	15.90390517	13.81772545	2.34646687	3.99883519
C	15.90390524	15.24441674	2.34557958	4.00116483
C	17.13948036	15.95777906	2.34646366	3.99883516
C	17.13948042	17.38447039	2.34557756	4.00116483
C	15.90390532	18.09783270	2.34646445	3.99883516
C	15.90390535	19.52452403	2.34557851	4.00116481
C	17.13948045	20.23788637	2.34646219	3.99883521
C	17.13948045	21.66457768	2.34557202	4.00116476
C	15.90390532	22.37793991	2.34645573	3.99883525
C	15.90390531	23.80463116	2.34556760	4.00116476
C	17.13948041	24.51799347	2.34645295	3.99883525
C	19.61063063	0.26404191	2.34557357	4.00116479
C	18.37505550	0.97740418	2.34646112	3.99883518
C	18.37505551	2.40409544	2.34557880	4.00116483
C	19.61063067	3.11745770	2.34646566	3.99883514
C	19.61063067	4.54414901	2.34557865	4.00116483
C	18.37505551	5.25751129	2.34646277	3.99883519
C	18.37505548	6.68420260	2.34557851	4.00116479
C	19.61063065	7.39756487	2.34646710	3.99883524
C	19.61063060	8.82425616	2.34558513	4.00116477
C	18.37505543	9.53761840	2.34647085	3.99883526
C	18.37505541	10.96430966	2.34558465	4.00116477
C	19.61063056	11.67767193	2.34647019	3.99883523
C	19.61063056	13.10436319	2.34558255	4.00116480
C	18.37505542	13.81772546	2.34646626	3.99883520
C	18.37505547	15.24441675	2.34557881	4.00116482
C	19.61063062	15.95777907	2.34646495	3.99883516
C	19.61063066	17.38447041	2.34557877	4.00116484
C	18.37505554	18.09783273	2.34646368	3.99883517
C	18.37505556	19.52452407	2.34557782	4.00116481
C	19.61063069	20.23788638	2.34646340	3.99883520
C	19.61063068	21.66457769	2.34557327	4.00116477
C	18.37505555	22.37793997	2.34645513	3.99883526
C	18.37505554	23.80463123	2.34556677	4.00116475
C	19.61063068	24.51799347	2.34645417	3.99883524

C	22.08178098	0.26404182	2.34557481	4.00116480
C	20.84620582	0.97740412	2.34646312	3.99883516
C	20.84620583	2.40409540	2.34558075	4.00116484
C	22.08178103	3.11745763	2.34646676	3.99883513
C	22.08178104	4.54414895	2.34557989	4.00116484
C	20.84620586	5.25751127	2.34646484	3.99883518
C	20.84620583	6.68420259	2.34558061	4.00116480
C	22.08178101	7.39756485	2.34646829	3.99883522
C	22.08178097	8.82425617	2.34558603	4.00116478
C	20.84620577	9.53761842	2.34647261	3.99883524
C	20.84620574	10.96430969	2.34558643	4.00116478
C	22.08178092	11.67767196	2.34647110	3.99883522
C	22.08178092	13.10436324	2.34558364	4.00116480
C	20.84620573	13.81772548	2.34646838	3.99883518
C	20.84620577	15.24441678	2.34558116	4.00116483
C	22.08178096	15.95777909	2.34646656	3.99883514
C	22.08178100	17.38447042	2.34558023	4.00116484
C	20.84620582	18.09783272	2.34646581	3.99883515
C	20.84620584	19.52452406	2.34557984	4.00116481
C	22.08178103	20.23788633	2.34646441	3.99883519
C	22.08178101	21.66457764	2.34557424	4.00116478
C	20.84620584	22.37793993	2.34645722	3.99883524
C	20.84620583	23.80463119	2.34556905	4.00116476
C	22.08178102	24.51799338	2.34645564	3.99883523
C	24.55293138	0.26404174	2.34557292	4.00116479
C	23.31735619	0.97740402	2.34646231	3.99883516
C	23.31735621	2.40409531	2.34557996	4.00116484
C	24.55293140	3.11745757	2.34646496	3.99883515
C	24.55293141	4.54414890	2.34557818	4.00116483
C	23.31735623	5.25751122	2.34646435	3.99883518
C	23.31735621	6.68420256	2.34558011	4.00116480
C	24.55293138	7.39756485	2.34646658	3.99883524
C	24.55293135	8.82425617	2.34558401	4.00116477
C	23.31735615	9.53761844	2.34647158	3.99883524
C	23.31735612	10.96430973	2.34558543	4.00116478

C	24.55293131	11.67767199	2.34646905	3.99883524
C	24.55293132	13.10436327	2.34558168	4.00116480
C	23.31735612	13.81772552	2.34646770	3.99883518
C	23.31735616	15.24441682	2.34558083	4.00116483
C	24.55293138	15.95777910	2.34646508	3.99883516
C	24.55293142	17.38447043	2.34557853	4.00116484
C	23.31735621	18.09783271	2.34646523	3.99883516
C	23.31735623	19.52452404	2.34557902	4.00116481
C	24.55293144	20.23788629	2.34646231	3.99883521
C	24.55293143	21.66457759	2.34557202	4.00116477
C	23.31735622	22.37793984	2.34645625	3.99883525
C	23.31735621	23.80463110	2.34556845	4.00116476
C	24.55293142	24.51799330	2.34645384	3.99883524
C	27.02408177	0.26404178	2.34557426	4.00116479
C	25.78850657	0.97740400	2.34646146	3.99883518
C	25.78850659	2.40409529	2.34557920	4.00116483
C	27.02408176	3.11745760	2.34646635	3.99883514
C	27.02408177	4.54414894	2.34557944	4.00116483
C	25.78850659	5.25751121	2.34646359	3.99883519
C	25.78850657	6.68420256	2.34557946	4.00116480
C	27.02408174	7.39756487	2.34646801	3.99883523
C	27.02408171	8.82425618	2.34558541	4.00116477
C	25.78850652	9.53761845	2.34647062	3.99883525
C	25.78850650	10.96430974	2.34558449	4.00116477
C	27.02408169	11.67767199	2.34647040	3.99883523
C	27.02408172	13.10436327	2.34558306	4.00116480
C	25.78850653	13.81772553	2.34646693	3.99883519
C	25.78850658	15.24441683	2.34558026	4.00116483
C	27.02408180	15.95777911	2.34646649	3.99883516
C	27.02408185	17.38447043	2.34557983	4.00116484
C	25.78850665	18.09783271	2.34646436	3.99883517
C	25.78850666	19.52452404	2.34557808	4.00116481
C	27.02408187	20.23788631	2.34646370	3.99883521
C	27.02408186	21.66457762	2.34557342	4.00116477
C	25.78850664	22.37793982	2.34645527	3.99883526

C	25.78850662	23.80463108	2.34556761	4.00116476
C	27.02408181	24.51799334	2.34645514	3.99883524
C	29.49523216	0.26404188	2.34557435	4.00116480
C	28.25965695	0.97740408	2.34646346	3.99883516
C	28.25965696	2.40409537	2.34558120	4.00116484
C	29.49523214	3.11745769	2.34646647	3.99883513
C	29.49523215	4.54414901	2.34557946	4.00116484
C	28.25965695	5.25751126	2.34646535	3.99883518
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C	30.73079591	0.96965970	5.59612254	3.99883520
C	29.49522094	1.68302262	5.59700281	4.00116482
C	29.49522084	3.10971397	5.59611615	3.99883516
C	30.73079610	3.82307581	5.59700639	4.00116480
C	30.73079604	5.24976704	5.59613202	3.99883521
C	29.49522101	5.96312952	5.59702251	4.00116478
C	29.49522101	7.38982063	5.59614692	3.99883522
C	30.73079623	8.10318249	5.59703738	4.00116475
C	30.73079625	9.52987362	5.59615359	3.99883524
C	29.49522120	10.24323599	5.59703606	4.00116476
C	29.49522119	11.66992717	5.59614498	3.99883521
C	30.73079637	12.38328911	5.59702792	4.00116477
C	30.73079631	13.80998029	5.59613264	3.99883520
C	29.49522129	14.52334288	5.59701222	4.00116482
C	29.49522108	15.95003412	5.59612160	3.99883515
C	30.73079628	16.66339595	5.59700825	4.00116482
C	30.73079610	18.09008720	5.59612522	3.99883517
C	29.49522112	18.80345003	5.59701194	4.00116482
C	29.49522090	20.23014137	5.59613350	3.99883518
C	30.73079613	20.94350323	5.59702472	4.00116477
C	30.73079592	22.37019464	5.59614416	3.99883526
C	29.49522093	23.08355762	5.59702767	4.00116478
C	29.49522078	24.51024910	5.59613591	3.99883524
C	30.73079605	25.22361103	5.59701782	4.00116478

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