

# **First-principles investigations on the functionalization of chiral and non-chiral carbon nanotubes by Diels-Alder cycloaddition reactions**

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## **Supporting Information**

**S1** (Pages 2-16): Cartesian coordinates and total energies of optimized structures discussed in the text

**S2** (Page 17): Molecular models of optimized structures discussed in the text

**S1:** Cartesian coordinates of optimized structures discussed in the text. The second line of the .xyz file reports the computed total energy in eV.

180				C	-0.010345	-0.103940	3.266353
-24436.312217				C	-0.013973	1.301161	3.017751
C	8.686206	-2.168796	2.776449	C	1.237361	1.962611	2.690835
C	8.681376	-0.908177	3.364641	C	1.250783	3.048402	1.768913
C	7.470116	-0.115772	3.394098	C	-0.026237	3.732533	1.287275
C	7.471678	1.318117	3.154465	C	-0.025630	3.964941	-0.335835
C	8.687885	2.049395	2.857008	C	1.250335	3.438693	-0.990113
C	8.695294	3.028261	1.870734	C	1.236589	2.640961	-2.170703
C	7.484055	3.328139	1.132513	C	-0.014311	2.090489	-2.661987
C	7.484092	3.527810	-0.305397	C	-0.010641	0.800328	-3.272072
C	8.695017	3.437960	-1.098127	C	1.239261	0.077795	-3.401724
C	8.686611	2.762131	-2.312257	C	1.242299	-1.346296	-3.200610
C	7.469605	2.138635	-2.794298	C	-0.005070	-2.004828	-2.876614
C	7.466899	0.819913	-3.406021	C	-0.003985	-3.034833	-1.880154
C	8.677702	0.048079	-3.590407	C	1.248824	-3.368774	-1.233539
C	8.683166	-1.323255	-3.356074	C	1.249095	-3.569135	0.193029
C	7.477587	-1.998480	-2.926869	C	-0.003613	-3.425265	0.906737
C	7.483029	-3.026827	-1.899831	C	-0.004670	-2.703083	2.144309
C	8.694885	-3.439906	-1.221405	C	-1.254718	-2.162039	2.633456
C	8.695345	-3.632580	0.155842	C	-1.257220	-0.842353	3.204383
C	7.483603	-3.420608	0.921689	C	-2.502828	-0.131223	3.307657
C	7.479112	-2.706311	2.187035	C	-2.511717	1.288174	3.048947
C	6.234107	-2.145705	2.643936	C	-1.271883	1.951155	2.691542
C	6.229893	-0.829235	3.249415	C	-1.293078	3.031941	1.768092
C	4.976288	-0.112501	3.322234	C	-2.539147	3.366096	1.147394
C	4.977717	1.300499	3.088845	C	-2.539080	3.572492	-0.305991
C	6.233124	1.949183	2.788050	C	-1.292457	3.424478	-0.994097
C	6.239893	2.981582	1.767212	C	-1.271592	2.630999	-2.174349
C	4.993522	3.311799	1.120365	C	-2.510964	2.086281	-2.696351
C	4.993548	3.509937	-0.296213	C	-2.501986	0.784782	-3.319663
C	6.239691	3.368102	-1.009482	C	-1.256969	0.071187	-3.406459
C	6.232065	2.649701	-2.271225	C	-1.254583	-1.352503	-3.203716
C	4.976166	2.105962	-2.733409	C	-2.500047	-2.010762	-2.895847
C	4.974056	0.804744	-3.331935	C	-2.500803	-3.044397	-1.884436
C	6.227067	0.093362	-3.452170	C	-1.256062	-3.372104	-1.233815
C	6.231898	-1.336371	-3.215797	C	-1.256019	-3.572707	0.192709
C	4.984204	-1.981551	-2.880758	C	-2.500847	-3.435796	0.907879
C	4.988747	-3.002640	-1.875131	C	-2.500478	-2.714316	2.161131
C	6.242747	-3.326002	-1.234732	C	-3.744007	-2.170839	2.645272
C	6.243226	-3.526773	0.201061	C	-3.745678	-0.859527	3.235105
C	4.989929	-3.390708	0.907106	C	-4.998538	-0.144259	3.332968
C	4.985929	-2.679136	2.150794	C	-5.008040	1.267829	3.093640
C	3.731618	-2.148195	2.639997	C	-3.762385	1.927392	2.756170
C	3.727528	-0.835370	3.225828	C	-3.775272	2.969002	1.765116
C	2.480896	-0.114266	3.300558	C	-5.036234	3.269175	1.114444
C	2.480951	1.306276	3.045855	C	-5.036190	3.468794	-0.302373
C	3.727631	1.954348	2.754850	C	-3.775000	3.359469	-1.009751
C	3.733326	2.999427	1.768650	C	-3.761801	2.624683	-2.245611
C	2.494920	3.389395	1.150197	C	-5.007165	2.078404	-2.747767
C	2.495121	3.594625	-0.302475	C	-4.997292	0.778980	-3.350118
C	3.733171	3.387771	-1.004362	C	-3.744658	0.062820	-3.442107
C	3.726869	2.648160	-2.236402	C	-3.743150	-1.357574	-3.218501
C	2.479675	2.101977	-2.688558	C	-4.995381	-2.004289	-2.888814
C	2.479535	0.798811	-3.309109	C	-4.997437	-3.019842	-1.877477
C	3.725467	0.082394	-3.427830	C	-3.747423	-3.360567	-1.231670
C	3.729903	-1.338727	-3.208941	C	-3.747635	-3.560810	0.192731
C	2.489395	-1.999650	-2.891631	C	-4.997946	-3.409879	0.906060
C	2.492538	-3.036142	-1.883257	C	-4.996506	-2.705740	2.154165
C	3.739954	-3.349462	-1.230630	C	-6.247073	-2.182181	2.651499
C	3.740437	-3.548963	0.193729	C	-6.248590	-0.867988	3.262466
C	2.493534	-3.426588	0.908223	C	-7.492689	-0.161773	3.409138
C	2.490645	-2.701216	2.159109	C	-7.502371	1.270650	3.161409
C	1.243259	-2.154901	2.631798	C	-6.267789	1.906428	2.789048
C	1.240196	-0.834574	3.201321	C	-6.281036	2.931265	1.760990
				C	-7.527213	3.267097	1.124348
				C	-7.527059	3.468694	-0.313693
				C	-6.280823	3.320807	-1.017676
				C	-6.267256	2.612373	-2.284672





C	6.829062	1.420677	-3.344218	C	-1.796637	1.341681	-3.320231
C	8.265106	1.441361	-3.364516	C	-0.365729	1.344400	-3.320246
C	4.676886	0.171717	-3.633542	C	-3.953643	0.137112	-3.659340
C	6.108927	0.186872	-3.617941	C	-2.519754	0.132248	-3.661228
C	6.835235	-1.036787	-3.426305	C	-1.796969	-1.112420	-3.544400
C	8.280577	-1.025343	-3.421067	C	-0.355393	-1.110292	-3.540321
C	4.691589	-2.201020	-2.955988	C	-3.957107	-2.233097	-2.999390
C	6.123214	-2.184335	-2.932558	C	-2.521540	-2.239711	-3.004631
C	6.854821	-3.063491	-2.036029	C	-1.795632	-3.099779	-2.087062
C	3.965784	-3.076722	-2.054412	C	-4.683481	-3.084103	-2.075002
C	0.362960	-3.568996	-0.925799	C	-8.276992	-3.492061	-0.884154
C	1.803994	-3.565451	-0.917059	C	-6.831498	-3.494793	-0.892841
C	2.521282	-3.613221	0.337072	C	-6.106611	-3.610567	0.344735
C	3.954306	-3.614705	0.347551	C	-4.675530	-3.616812	0.333062
C	0.358960	-3.190238	1.509442	C	-8.268495	-3.253202	1.575473
C	1.795028	-3.203968	1.522904	C	-6.830250	-3.264597	1.555698
C	2.508219	-2.441939	2.513414	C	-6.110394	-2.486443	2.532664
C	3.948126	-2.455632	2.531193	C	-4.666389	-2.461750	2.511827
C	0.356057	-1.340820	3.145284	C	-8.274508	-3.492579	3.268039
C	1.786482	-1.382776	3.188760	C	-6.837701	-1.460996	3.238370
C	2.513909	-0.187736	3.532610	C	-6.120789	-0.227497	3.512937
C	3.954680	-0.202487	3.553068	C	-4.682282	-0.203111	3.509844
C	0.366901	1.104502	3.515100	C	-8.294016	0.977495	3.360787
C	1.801422	1.063621	3.491703	C	-6.851325	0.992895	3.372119
C	2.545464	2.208592	2.994105	C	-6.136477	2.165218	2.919493
C	3.962437	2.183384	2.960582	C	-4.720949	2.198079	2.970652
C	0.369816	3.064245	2.107570	C	-8.301277	3.025495	1.986139
C	1.795055	3.044696	2.053194	C	-6.867737	3.028850	1.998476
C	2.508589	3.433356	0.862094	C	-6.130088	3.461897	0.840279
C	3.952729	3.450209	0.847663	C	-4.681111	3.441589	0.856623
C	0.349880	3.410659	-0.343080	C	-8.274236	3.564944	-0.428415
C	1.780077	3.460968	-0.375757	C	-6.836792	3.534670	-0.412649
C	2.499770	3.126070	-1.592472	C	-6.099461	3.131841	-1.599911
C	3.932163	3.152619	-1.608548	C	-4.668102	3.116502	-1.590820
C	0.348773	2.357420	-2.581857	C	-8.261409	2.378463	-2.593246
C	1.785971	2.379093	-2.597036	C	-6.816313	2.360293	-2.577399
C	2.511702	1.368745	-3.326775	C	-6.104065	1.357702	-3.322637
C	3.943729	1.385408	-3.329418	C	-4.673569	1.353493	-3.325877
C	0.363276	0.136861	-3.655123	C	-8.277258	0.163126	-3.680359
C	1.797174	0.146248	-3.648287	C	-6.840328	0.152832	-3.665893
C	2.524933	-1.092137	-3.516331	C	-6.125438	-1.091597	-3.525506
C	3.965963	-1.078062	-3.500535	C	-4.679441	-1.101016	-3.531137
C	0.369489	-2.236347	-2.997134	C	-8.288189	-2.211425	-2.990627
C	1.805041	-2.227406	-2.985852	C	-6.851315	-2.215266	-2.988887
C	2.529765	-3.086665	-2.067748	C	-6.118072	-3.063657	-2.061756
C	-0.357919	-3.099855	-2.085379	C	-9.009366	-3.118954	-2.067707
C	-3.959794	-3.558692	-0.920689	C	-11.066048	-3.871501	-0.958590
C	-2.517731	-3.565997	-0.927676	C	-10.387398	-3.962407	-0.279691
C	-1.793425	-3.609167	0.321396	C	-8.994601	-3.702941	0.348149
C	-0.361452	-3.607923	0.322587	C	-8.955480	-2.507455	2.540061
C	-3.949241	-3.219397	1.523873	C	-10.405486	-0.171765	3.862788
C	-2.513654	-3.198589	1.510393	C	-9.007522	-0.248751	3.609129
C	-1.797953	-2.393872	2.463114	C	-11.080285	1.061218	3.736919
C	-0.359449	-2.389054	2.462579	C	-10.419255	2.193493	3.195626
C	-3.948576	-1.399037	3.184444	C	-9.027479	2.148264	2.943443
C	-2.519273	-1.349297	3.143418	C	-8.976550	3.440117	0.803198
C	-1.816650	-0.112925	3.449747	C	-10.373390	3.428224	-1.910003
C	-0.353161	-0.110443	3.454769	C	-8.985361	3.232672	-1.686303
C	-3.976720	1.052165	3.462935	C	-11.038966	2.695246	-2.919660
C	-2.541216	1.099086	3.498919	C	-10.377453	1.647410	-3.602156
C	-1.892180	2.503174	3.396429	C	-8.989098	1.434734	-3.403478
C	-0.285149	2.505339	3.400479	C	-8.971537	-1.062151	-3.481637
C	-3.968210	3.052472	2.047150	C	-10.406422	-3.370405	-2.103971
C	-2.543256	3.071241	2.105219	H	10.077958	-3.400290	-0.831139
C	-1.814637	3.364104	0.919947	H	10.956320	-4.197522	1.202721
C	-0.355362	3.359697	0.920763	H	12.130203	-2.927649	3.030845
C	-3.948843	3.467399	-0.377924	H	10.953131	-1.034225	4.203122
C	-2.518788	3.414985	-0.344070	H	10.076408	0.959554	3.297088
C	-1.799132	3.054466	-1.547251	H	10.976380	3.123631	2.949168
C	-0.369593	3.055891	-1.547386	H	12.131619	4.080944	0.927987
C	-3.953537	2.363812	-2.590718	H	10.936422	4.158335	-1.285765
C	-2.515313	2.350169	-2.578944	H	10.051883	2.399479	-2.566439

H	10.955278	1.023701	-4.243689	C	6.102474	3.537375	-0.470066
H	12.150614	-1.180991	-4.037094	C	6.832796	3.210091	-1.684633
H	10.987393	-3.150988	-2.988126	C	8.269404	3.237706	-1.697887
H	-12.150214	-4.106143	-1.007936	C	4.671226	2.435273	-2.675061
H	-10.952252	-4.209487	1.203186	C	6.116967	2.445846	-2.675608
H	-10.061909	-2.455449	2.480064	C	6.843553	1.418330	-3.378062
H	-10.969882	-1.085196	4.145481	C	8.280446	1.431580	-3.388707
H	-12.162856	1.121494	3.976497	C	4.684508	0.179467	-3.665233
H	-11.002327	3.104364	2.944153	C	6.116765	0.187059	-3.644205
H	-10.080936	3.338580	0.767209	C	6.837002	-1.039079	-3.434629
H	-10.941750	4.143759	-1.279250	C	8.283218	-1.035852	-3.427806
H	-12.115597	2.883129	-3.114913	C	4.685248	-2.182056	-2.949172
H	-10.950287	0.979495	-4.279415	C	6.118170	-2.175190	-2.928558
H	-10.075594	-1.025340	-3.379101	C	6.846307	-3.051942	-2.024660
H	-10.985814	-3.153484	-3.025906	C	3.956537	-3.042946	-2.037236
C	-2.422150	3.363207	4.619689	C	0.360642	-3.512166	-0.892608
C	-1.776018	4.723346	4.652651	C	1.799007	-3.511438	-0.888240
C	-0.417810	4.728851	4.651782	C	2.517507	-3.561328	0.363846
C	0.239602	3.374456	4.619420	C	3.951047	-3.570752	0.368597
H	0.186268	5.660787	4.650546	C	0.365228	-3.160814	1.547595
H	-2.387557	5.650461	4.652079	C	1.794034	-3.166318	1.554673
H	-2.179951	2.796602	5.559047	C	2.510880	-2.402206	2.554261
H	-3.532615	3.428264	4.576186	C	3.956039	-2.424805	2.560256
H	1.348881	3.449673	4.572419	C	0.357702	-1.331783	3.220016
H	0.006313	2.808101	5.561283	C	1.795741	-1.372589	3.257738
				C	2.533290	-0.162995	3.599432
				C	3.969792	-0.179958	3.579080
				C	0.359885	1.170687	3.887156
<b>1@ (9,0), site b:</b>				C	1.833931	1.081263	3.519348
				C	2.535783	2.172866	2.933800
214				C	3.970279	2.165988	2.893433
-29182.991097				C	0.368536	2.984068	1.984426
C	8.964733	-3.501594	-0.854777	C	1.785393	2.994892	1.973350
C	8.994738	-3.290824	1.632566	C	2.509928	3.417752	0.795634
C	10.384951	-3.480449	1.844597	C	3.953482	3.445970	0.788345
C	11.058477	-2.733058	2.839135	C	0.361888	3.456434	-0.441211
C	9.009319	-1.470668	3.325180	C	1.791568	3.479496	-0.450223
C	10.400533	-1.678698	3.514084	C	2.514337	3.157921	-1.666895
C	8.985987	1.029555	3.374260	C	3.946464	3.173016	-1.670660
C	9.009556	3.083876	1.949307	C	0.357325	2.414294	-2.674741
C	10.401179	3.358091	1.988593	C	1.796545	2.421380	-2.678155
C	11.059283	3.854769	0.838913	C	2.521080	1.394641	-3.387953
C	8.992384	3.649658	-0.470648	C	3.954719	1.401133	-3.382189
C	10.383972	3.921846	-0.401569	C	0.364283	0.168666	-3.690283
C	8.961367	2.443898	-2.656202	C	1.799094	0.171016	-3.685466
C	9.007127	0.178795	-3.708515	C	2.523408	-1.068764	-3.525679
C	10.402415	0.090014	-3.952651	C	3.965169	-1.063610	-3.511495
C	11.072464	-1.145905	-3.796657	C	0.365039	-2.191241	-2.976354
C	9.008182	-2.201051	-2.987162	C	1.800472	-2.189149	-2.970586
C	10.403860	-2.260973	-3.240194	C	2.523553	-3.043754	-2.046239
C	8.283048	-3.067212	-2.026635	C	-0.361533	-3.043696	-2.054033
C	4.674770	-3.511513	-0.874713	C	-3.954427	-3.502949	-0.877781
C	6.120663	-3.518626	-0.870268	C	-2.515044	-3.507651	-0.887277
C	6.836526	-3.602907	0.377999	C	-1.791430	-3.562319	0.359606
C	8.273303	-3.630838	0.382197	C	-0.358650	-3.558847	0.356643
C	4.672230	-3.194126	1.571911	C	-3.939102	-3.199725	1.573823
C	6.105380	-3.200876	1.569037	C	-2.510427	-3.187557	1.560988
C	6.829226	-2.414298	2.530445	C	-1.787837	-2.403844	2.539359
C	8.275619	-2.428227	2.535868	C	-0.354873	-2.379318	2.524107
C	4.685125	-1.400506	3.266231	C	-3.942299	-1.402466	3.265388
C	6.118999	-1.403163	3.261687	C	-2.506149	-1.376767	3.244948
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C	8.296857	-0.197387	3.590183	C	-0.368243	-0.150361	3.607499
C	4.698291	1.051195	3.437776	C	-3.974609	1.056587	3.430394
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C	8.297016	2.172835	2.878086	C	-0.365931	2.458311	3.222954
C	4.686438	3.004597	1.950728	C	-3.971896	3.007301	1.946207
C	6.118009	2.999988	1.940587	C	-2.536200	3.009576	1.971496
C	6.827642	3.425609	0.765334	C	-1.798385	3.439949	0.803778
C	8.274281	3.439405	0.760831	C	-0.351730	3.375832	0.812791
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C	-6.049551	-3.296226	-1.929722	C	-4.440679	-0.115759	3.889962
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C	-2.352144	-2.741381	-2.669163	C	1.853156	0.294295	3.994960
C	-3.554446	-3.223451	-2.040846	C	0.577359	-0.348163	3.963663
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C	2.310793	2.682980	-2.613477	C	-5.782574	-2.090869	3.195853
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C	3.907208	-2.970177	-2.307344	C	0.489802	-1.666811	3.432570
C	4.795321	2.781036	-2.505919	C	-0.795476	-2.225096	3.059899
C	3.509012	3.171001	-1.981432	C	2.975023	-1.840132	3.401058
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C	7.283759	2.924289	-2.438747	C	4.179217	-2.489158	2.941919
C	6.002635	3.257546	-1.872165	C	7.909349	-2.136668	3.455004
C	8.860878	-2.902981	-2.476364	C	6.671777	-2.650713	2.929115
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C	-6.499388	3.553647	-1.182398	C	-5.841385	-3.118054	2.180100
C	-7.779259	3.764418	-0.547730	C	-7.112169	-3.510017	1.626870
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C	-0.337004	3.691905	-0.100788	C	4.108214	-3.355021	1.799767
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C	4.634923	3.760878	0.147806	C	7.776588	-3.777063	0.951092
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C	-7.846754	3.793010	0.871016	C	-4.687692	-3.783009	0.093894
C	-5.398188	3.648264	1.033873	C	-5.973547	-3.768834	-0.564832
C	-6.694761	3.501848	1.660272	C	-2.204976	-3.768585	-0.029105
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C	5.779501	3.136155	2.248810	C	8.918846	-3.612148	-1.284916
C	8.224117	3.122429	2.446495	H	9.697546	-0.686349	-3.977717
C	-6.777007	2.665944	2.869701	H	9.552523	1.762139	-3.736986
C	-8.023877	2.132516	3.352103	H	-9.484695	-3.457642	-2.326078
C	-4.281243	2.528907	2.946596	H	-9.592821	-1.777229	-3.774835
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C	-1.804856	2.453776	3.103722	H	-9.727368	0.667968	-4.029445
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C	0.732924	2.358841	3.202656	H	9.438082	3.421938	-2.267736
C	-0.580536	2.018970	3.898243	H	9.303879	4.195963	0.065919
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C	5.707702	2.119495	3.278119	H	9.219661	3.522157	2.164656
C	4.421690	1.552521	3.611510	H	-8.967025	2.693834	3.188875
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C	6.909983	1.444142	3.688898	H	-9.102090	0.406605	4.073463
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C	-5.660818	0.658542	3.831093	H	-9.174376	-1.784183	3.801251
C	-6.933629	-0.007926	3.898709	H	8.847591	-2.714510	3.326181
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C	1.269274	-0.654335	-3.800621	C	4.537425	3.470376	1.490441
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C	-0.099790	1.410915	-3.597844	C	7.034415	3.515984	1.643902
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C	-1.222091	-0.793247	-3.787173	C	8.202717	3.159441	2.411170
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C	5.315507	-3.637588	1.044607	C	-1.214888	-0.793859	-3.775757
C	7.768432	-3.798746	0.919308	C	0.069847	-1.423330	-3.574225
C	-7.178617	-3.880431	0.172657	C	-2.580412	1.279592	-3.616231
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C	-4.685682	-3.775884	0.059410	C	-3.708029	-0.922836	-3.747200
C	-5.971468	-3.766407	-0.602890	C	-2.423329	-1.546887	-3.538901
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H	9.807448	-2.668893	-3.034580	C	-3.554874	-3.209449	-2.088810
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H	9.286877	4.230918	0.039002	C	-3.942099	2.938556	-2.359258
H	-8.851727	3.808125	1.307050	C	0.141867	-2.627127	-2.784825
H	-9.957437	3.941366	-1.013187	C	-1.068175	-3.135105	-2.189454
H	9.194329	3.580608	2.145710	C	-0.169281	2.604616	-2.763134
H	-8.964024	2.701539	3.157719	C	-1.454129	3.026979	-2.264897
H	9.087092	1.790342	3.828395	C	2.633795	-2.526976	-2.842975
H	-9.112821	0.411377	4.031669	C	1.422271	-3.053510	-2.267242
H	9.004475	-0.408792	4.124613	C	2.320331	2.700954	-2.646390
H	-9.195800	-1.783312	3.735028	C	1.031272	3.106404	-2.140739
H	8.863935	-2.700963	3.255481	C	5.124191	-2.411701	-2.884416
H	-9.286110	-3.575935	2.053712	C	3.910769	-2.966260	-2.333513
H	8.768566	-3.806000	1.400287	C	4.805292	2.787937	-2.518120
H	-9.351267	-4.267694	-0.050672	C	3.516733	3.185394	-2.007450
H	9.894374	-3.948169	-0.910198	C	7.622868	-2.330089	-2.958609
C	-0.967016	1.065388	5.851877	C	6.407338	-2.871892	-2.405364
C	0.268649	1.244083	6.698096	C	7.296308	2.928387	-2.438858
C	1.127972	0.193188	6.760627	C	6.011601	3.261355	-1.878043
C	0.817576	-0.986373	5.869869	C	8.872468	-2.903304	-2.492984
H	2.063939	0.223822	7.357215	C	8.453676	3.477158	-1.772749
H	0.437741	2.189757	7.256100	C	-6.498172	3.554786	-1.200524
H	-1.642840	0.336451	6.370435	C	-7.778037	3.770033	-0.561620
H	-1.553496	2.010241	5.751603	C	-8.962489	3.625908	-1.389383
H	1.640943	-1.739242	5.866244	C	-4.017016	3.576695	-1.073746
H	-0.114112	-1.517651	6.201194	C	-5.299996	3.713039	-0.424836
				C	-1.533082	3.614792	-0.949970
				C	-2.814420	3.706070	-0.295013
				C	0.948130	3.651515	-0.810463
				C	-0.335667	3.722063	-0.164264

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C	7.487290	3.520758	-0.304681	C	-2.511253	1.296699	3.063372
C	7.488844	3.324191	1.134121	C	-1.271009	1.961337	2.707307
C	6.244034	2.981836	1.771092	C	-1.291251	3.041172	1.781491
C	6.237522	1.954026	2.797198	C	-2.538148	3.364400	1.155516
C	7.476209	1.324116	3.166599	C	-2.537269	3.553358	-0.300388
C	8.692781	2.055189	2.867074	C	-1.291790	3.394610	-0.987307
C	8.700004	3.028069	1.874713	C	-1.270730	2.608086	-2.170596
C	4.981064	1.308197	3.101254	C	-2.510398	2.070197	-2.695942
C	4.979625	-0.105106	3.335219	C	-2.501774	0.774748	-3.330347
C	6.233367	-0.822378	3.261354	C	-1.256297	0.061170	-3.422252
C	7.474550	-0.109798	3.408049	C	-1.253613	-1.361740	-3.218569
C	6.238106	-2.137313	2.651931	C	-2.499318	-2.017689	-2.905541
C	7.483549	-2.697068	2.193597	C	-2.498981	-3.041915	-1.885405
C	8.691142	-2.161534	2.785605	C	-1.253565	-3.363426	-1.232986
C	8.686122	-0.902610	3.378010	C	-1.253312	-3.555692	0.094279
C	6.233855	2.641454	-2.270019	C	-2.498131	-3.419303	0.909571
C	7.472481	2.136449	-2.797585	C	-2.497910	-2.701344	2.164578
C	8.688093	2.766250	-2.317654	C	-3.742222	-2.161845	2.651699
C	8.696392	3.438378	-1.101286	C	-3.744726	-0.852964	3.246635
C	4.978402	2.097131	-2.733555	C	-4.999091	-0.139807	3.345722
C	4.978119	0.798932	-3.339500	C	-5.009090	1.272886	3.106696
C	6.232405	0.090126	-3.460294	C	-3.763329	1.933676	2.770131
C	7.472214	0.818604	-3.412425	C	-3.775384	2.970462	1.773580
C	6.238458	-1.339498	-3.222033	C	-5.036378	3.264123	1.119176
C	7.484850	-1.998472	-2.928356	C	-5.035029	3.455237	-0.298733
C	8.691484	-1.322587	-3.357781	C	-3.772831	3.340698	-1.003795
C	8.684705	0.048456	-3.594938	C	-3.760327	2.608358	-2.241350
C	4.989816	-1.984445	-2.886450	C	-5.005888	2.067769	-2.746808
C	4.993757	-2.998491	-1.873756	C	-4.997386	0.771799	-3.357251
C	6.247647	-3.318437	-1.230895	C	-3.744971	0.054542	-3.454190
C	7.489122	-3.022539	-1.896951	C	-3.743187	-1.3265390	-3.229705
C	6.247211	-3.514836	0.205733	C	-4.995726	-2.008847	-2.894560
C	7.488355	-3.409484	0.926706	C	-4.996371	-3.017480	-1.876397
C	8.700545	-3.623187	0.161260	C	-3.745602	-3.353134	-1.229532
C	8.700704	-3.433593	-1.216617	C	-3.744970	-3.546780	0.195504
C	4.993108	-3.376679	0.910925	C	-4.995385	-3.398060	0.909538
C	4.988954	-2.668038	2.156578	C	-4.994343	-2.697375	2.159720
C	3.734215	-2.137273	2.647028	C	-6.246126	-2.177690	2.658831
C	3.729782	-0.826492	3.237579	C	-6.248603	-0.864864	3.273300
C	2.483032	-0.104589	3.313714	C	-7.494104	-0.159639	3.419012
C	2.483195	1.316399	3.059937	C	-7.504369	1.273035	3.170080
C	3.731236	1.962485	2.767570	C	-6.269362	1.908931	2.798339
C	3.728540	2.633283	-2.232915	C	-6.282012	2.929055	1.765447
C	2.482377	2.086610	-2.688769	C	-7.527813	3.261921	1.176388
C	2.482443	0.788924	-3.320063	C	-7.526282	3.460113	-0.312089
C	3.729639	0.075085	-3.440373	C	-6.279128	3.308196	-1.014194
C	3.734648	-1.345434	-3.220596	C	-6.265310	2.601811	-2.282520
C	2.493083	-2.005603	-2.901377	C	-7.500278	2.092834	-2.814664
C	2.496111	-3.032773	-1.884376	C	-7.491751	0.777950	-3.435440
C	3.743584	-3.340934	-1.228233	C	-6.247808	0.056480	-3.480687
C	3.743277	-3.533770	0.196844	C	-6.246551	-1.372291	-3.235904
C	2.495881	-3.409232	0.910631	C	-7.489958	-2.035708	-2.939791
C	2.492532	-2.687036	2.162906	C	-7.491395	-3.051536	-1.900534
C	1.244982	-2.141597	2.637264	C	-6.249240	-3.340040	-1.232865
C	1.241840	-0.823873	3.212489	C	-6.248592	-3.537939	0.203287
C	-0.009092	-0.093836	3.279372	C	-7.490620	-3.441897	0.924247
C	-0.012749	1.311791	3.033036	C	-7.488858	-2.740851	2.197258
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C	1.238639	2.617875	-2.166966	C	-8.701065	-0.959852	3.390332
C	-0.012995	2.071449	-2.661202	C	-8.737910	2.960783	1.866630
C	-0.009402	0.788610	-3.284477	C	-8.725620	1.993025	2.863888
C	1.241733	0.068125	-3.418039	C	-8.720402	2.709727	-2.330640
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C	-0.003018	-2.011689	-2.888052	C	-8.698887	-1.369881	-3.775540
C	-0.001337	-3.031633	-1.882397	C	-8.699227	-0.000063	-3.620767
C	1.251627	-3.359732	-1.232380	C	-8.702126	-3.653557	0.157861
C	1.251628	-3.551654	0.194791	C	-8.702516	-3.462212	-1.219672
C	-0.001211	-3.406847	0.908136	H	9.650096	-0.457786	3.701547
C	-0.002638	-2.687791	2.147014	H	9.655375	1.747660	3.326557
C	-1.252769	-2.149518	2.638662	H	9.667306	3.474801	1.563038
C	-1.255749	-0.832542	3.215390	H	9.663369	3.791413	-0.685260
C	-2.502422	-0.123102	3.320556	H	9.649469	2.598685	-2.846851

H	9.647342	0.565630	-3.789412	C	-0.355784	-3.045560	5.648036
H	9.659616	-1.865247	-3.367900	C	-1.703497	-2.895157	5.169425
H	9.665478	-3.461975	-1.764772	C	-2.263240	-3.928406	4.368111
H	9.665501	-3.798244	0.681468	C	-1.431821	-4.932536	3.792728
H	9.658182	-2.688921	2.648901	C	0.023712	-0.628599	5.417301
H	-9.667407	-0.522127	3.716856	C	-1.326076	-0.469347	4.924590
H	-9.686796	1.681457	3.323750	C	-2.285939	-1.533463	5.081819
H	-9.708392	3.398750	1.551696	C	-1.677987	0.685727	4.137477
H	-9.704538	3.714251	-0.691525	C	-3.053969	0.946111	3.903649
H	-9.680494	2.537399	-2.860753	C	-4.032973	0.017774	4.327078
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H	-9.663680	-1.918656	-3.389541	C	1.039252	0.318111	5.049908
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H	-9.667689	-3.827223	0.677418	C	-0.557628	1.296903	3.382218
H	-9.663137	-2.749100	2.656057	C	0.680803	-5.462509	1.999018
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H	0.063786	5.594050	-1.804034	C	-1.774734	-5.447802	2.446374
H	0.066163	5.010922	3.101259	C	-0.928372	-5.270494	0.116436
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C	1.995952	7.075925	-0.563998	C	-3.316443	-5.644271	0.546160
C	2.921349	7.783019	0.236181	C	-3.094941	-5.580623	1.940803
C	2.879393	7.661153	1.644740	C	1.788189	-5.468017	1.095039
C	1.928009	6.812445	2.255733	C	1.519784	-4.735979	-0.129563
C	0.989620	6.114059	1.461054	C	0.171234	-4.596953	-0.616116
H	2.031881	7.160392	-1.671743	C	3.131597	-5.613044	1.573449
H	3.682303	8.436082	-0.242944	C	3.371126	-5.969041	2.952326
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H	1.906622	6.701260	3.361940	C	3.897285	-3.970681	-0.096314
				C	4.226692	-5.009044	0.838624
				C	2.105211	-2.552354	-1.110423
				C	0.761350	-2.396615	-1.580406
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				C	4.833560	-2.865712	-0.198272
				C	6.176836	-3.023079	0.230627
				C	2.135975	-0.216481	-0.343992
				C	0.781493	-0.049152	-0.822779
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				C	-1.689559	0.502186	-2.053509
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				C	2.631872	0.613422	0.719228
				C	1.636165	1.271222	1.550418
				C	0.295763	1.461862	1.066098
				C	3.974863	0.443385	1.190199
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				C	6.962893	-1.859888	0.654461
				C	1.902105	1.301259	2.966657
				C	3.252710	1.122783	3.451510
				C	4.332004	0.900949	2.520505
				C	5.669358	0.714880	3.002150
				C	6.662509	0.066176	2.163030
				C	-0.758072	1.617009	2.009448
				C	2.373733	0.164190	5.547915
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				C	4.818796	0.599787	5.317153
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				C	2.687134	-0.916275	6.453218
				C	4.030623	-1.070642	6.953322
				C	5.062692	-0.153792	6.534143
				C	8.760492	-6.505009	4.880403
				C	9.019287	-6.531978	6.294816
				C	9.873250	-6.277725	3.995676
				C	8.313783	-2.035195	1.081144
				C	7.993029	-0.146446	2.648114
				C	8.866766	-1.104159	2.003271
				C	10.235018	-1.255310	2.489458
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C	10.496646	-3.558440	1.264832	C	0.781493	-0.049152	-0.822779
C	11.479610	-3.833168	0.062680	C	0.196760	-1.029948	-1.702579
C	11.353895	-2.764902	-0.987411	C	-0.043970	1.012088	-0.305036
C	7.980047	-4.417337	1.255505	C	-1.254420	1.315516	-0.981880
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C	10.694379	-4.719797	2.266824	C	2.631872	0.613422	0.719228
C	7.182771	-5.952079	3.026571	C	1.636165	1.271222	1.550418
C	5.837923	-5.857702	2.543769	C	0.295763	1.461862	1.066098
C	5.578944	-5.139738	1.321771	C	3.974863	0.443385	1.190199
C	6.619054	-4.277845	0.817793	C	4.843173	-0.522828	0.562134
C	4.721723	-6.101906	3.435302	C	6.194883	-0.701728	1.042288
C	4.983574	-6.073019	4.849725	C	6.962893	-1.859888	0.654461
C	6.330695	-6.209775	5.329559	C	1.902105	1.301259	2.966657
C	7.415315	-6.340122	4.395731	C	3.252710	1.122783	3.451510
C	3.967047	-5.501904	5.711261	C	4.332004	0.900949	2.520505
C	4.429026	-4.705051	6.825184	C	5.669358	0.714880	3.002150
C	5.776890	-4.857453	7.313234	C	6.662509	0.066176	2.163030
C	6.667768	-5.800398	6.679097	C	-0.758072	1.617009	2.009448
C	3.686153	-3.505178	7.122542	C	2.373733	0.164190	5.547915
C	4.459196	-2.336854	7.502960	C	3.481494	0.767887	4.831850
C	5.799744	-2.490492	7.994188	C	4.818796	0.599787	5.317153
C	6.385863	-3.814146	8.104154	C	5.933696	0.768187	4.417565
C	8.008331	-5.956154	7.159356	C	2.687134	-0.916275	6.453218
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C	7.732745	-3.968038	8.583876	C	5.062692	-0.153792	6.534143
C	2.345581	-3.352812	6.629334	C	8.760492	-6.505009	4.880403
C	1.737757	-4.398038	5.844088	C	9.019287	-6.531978	6.294816
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C	2.285968	-5.798713	3.889524	C	8.313783	-2.035195	1.081144
C	0.942591	-5.647563	3.410560	C	7.993029	-0.146446	2.648114
C	-0.082294	-5.067412	4.265638	C	8.866766	-1.104159	2.003271
C	0.386038	-4.246162	5.354516	C	10.235018	-1.255310	2.489458
C	1.766503	-2.027487	6.504614	C	11.043874	-2.342858	2.059837
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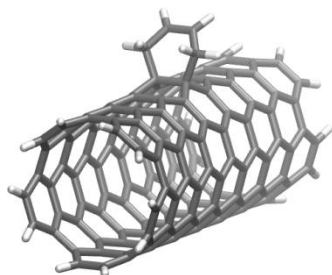
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C	9.356567	7.182602	-8.025089	C	3.541161	5.420801	-10.590677
C	8.143849	7.930073	-8.256053	C	2.584002	6.246655	-11.285104
C	7.833415	9.040803	-7.392605	C	2.632043	7.635750	-11.177022
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C	7.083835	7.339100	-9.034384	C	17.056453	3.027758	-4.615843
C	5.877227	8.088059	-9.276968	C	10.085410	3.647769	-7.137129
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C	4.805853	7.496958	-10.048080	C	5.487123	3.997975	-8.993428
C	3.632944	8.273523	-10.355962	C	6.420098	3.369046	-8.092888
C	3.344538	9.442979	-9.539238	C	3.188839	4.149909	-9.971198
C	4.229610	9.739662	-8.441824	C	4.104992	3.567191	-9.025109
C	3.678019	10.228971	-7.199344	C	13.851679	1.414602	-3.422079
C	2.255016	10.439803	-7.085698	C	15.266897	1.529491	-3.640715
C	1.518523	10.564648	-8.321983	C	8.251986	2.351987	-6.079598
C	2.046035	10.073253	-9.513527	C	5.921907	2.583770	-6.993062
C	5.924863	9.993533	-6.118367	C	6.803292	2.220929	-5.901540
C	4.492969	10.136442	-6.008220	C	3.594034	2.840265	-7.887645
C	3.849315	9.784858	-4.774992	C	4.498261	2.514418	-6.805667
C	2.416794	9.594219	-4.763239	C	2.172366	2.758087	-7.678935
C	1.604528	10.138110	-5.822410	C	1.337497	2.987791	-8.831014
C	8.160379	9.737943	-5.033200	C	1.835358	3.651967	-9.952488
C	6.724895	9.873766	-4.924287	C	13.359762	1.257607	-2.073274
C	6.076193	9.470896	-3.702158	C	14.281907	1.192473	-0.970001
C	4.650805	9.250889	-3.702382	C	15.643153	0.856534	-1.295433
C	10.389360	9.459333	-3.945308	C	16.121490	1.027767	-2.596518
C	8.956137	9.585507	-3.838782	C	11.963899	1.533704	-1.820716
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C	17.640366	8.429974	-1.962632	C	5.788165	3.709848	-2.381815
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C	15.623367	8.640275	-0.562127	C	3.455349	4.105431	-3.197156
C	14.967206	8.058596	0.599367	C	1.117654	4.487891	-4.025636
C	13.563621	7.748786	0.507931	C	0.055869	4.019007	-4.877415
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C	15.209758	6.271871	2.279257	C	13.721047	4.260733	1.796790
C	15.701282	7.424463	1.667853	C	14.758072	3.298078	2.076032
C	17.290144	4.405718	-4.884387	C	14.853772	2.121033	1.333345
C	18.492023	5.087664	-4.448180	C	10.302547	4.187111	0.096355
C	18.435359	6.422273	-4.059765	C	11.477913	4.680113	0.769134
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C	11.729435	6.093705	0.798273	C	9.230930	5.097072	-0.218355
C	8.577236	7.396831	-0.885650	C	5.779357	5.020369	-1.780292
C	9.491997	6.511335	-0.204781	C	6.977777	5.518555	-1.167162
C	11.622397	5.588135	-7.254824	C	3.473566	5.432186	-2.629629
C	6.341517	7.801284	-1.890873	C	4.701802	5.934364	-2.073484
C	7.250062	6.938281	-1.186133	C	1.146236	5.852934	-3.476570
C	9.340384	5.754963	-8.221026	C	2.415247	6.349419	-2.975298
C	10.396946	4.957993	-7.663611	C	0.142303	6.809123	-3.800747
C	4.102354	8.186556	-2.900361	H	0.466152	10.917110	-8.309686
C	5.002543	7.341201	-2.166210	H	1.398203	10.049556	-10.414474
C	7.054304	5.906772	-9.194569	H	16.729273	7.742623	1.914353
C	8.102659	5.117227	-8.602866	H	17.714517	8.724356	0.174763
C	1.862556	8.577311	-3.906408	H	19.331071	6.883790	-3.594368
C	2.752771	7.738800	-3.149583	H	18.742784	8.317436	-2.024147
C	4.764421	6.058158	-10.177791	H	-0.507521	10.551639	-6.369961

H	1.805249	8.233992	-11.612727	H	5.909692	-0.094653	-3.463530
H	1.721172	5.781028	-11.805269	H	5.528449	0.930482	-2.048988
H	17.875986	2.453001	-4.135799	H	9.703830	-0.534439	-4.236429
H	19.424090	4.504245	-4.288981	H	7.942125	-0.570227	-4.604069
H	1.131140	3.924824	-10.765415	C	6.983031	-0.777630	-0.508319
H	17.209921	0.909476	-2.779102	C	7.844191	-1.684638	0.150083
H	0.253173	2.754413	-8.788029	C	8.992625	-2.177895	-0.511533
H	16.365609	0.607609	-0.490623	C	9.297610	-1.746012	-1.823556
H	-0.500338	2.991997	-6.695918	C	8.432970	-0.847573	-2.489332
H	15.745556	1.474360	1.468729	H	6.078832	-0.386390	0.006576
H	-0.974370	4.410713	-4.746564	H	7.619701	-2.004531	1.189486
H	15.578123	3.551512	2.779663	H	9.663740	-2.895877	0.005011
H	-0.872727	6.470507	-4.096065	H	10.215336	-2.109568	-2.335006
H	15.859743	5.729588	2.997157				
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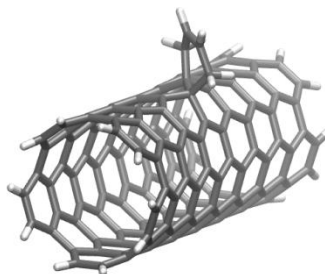


**S2:** Molecular models of optimized structures discussed in the text

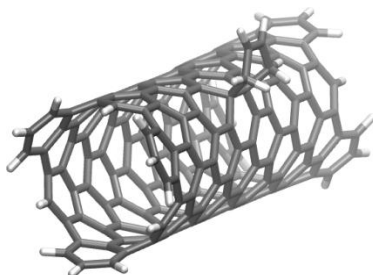
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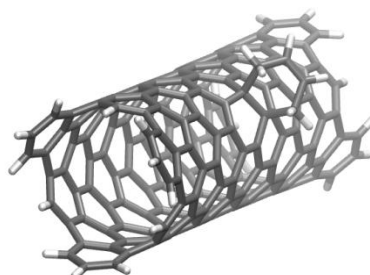
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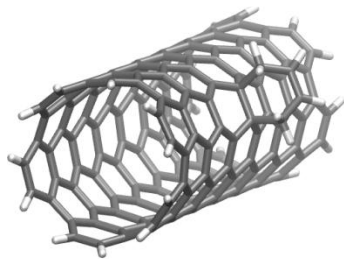
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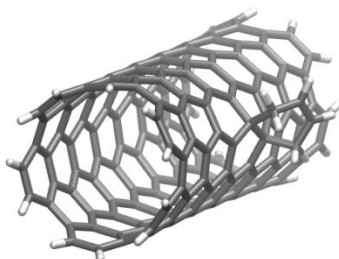
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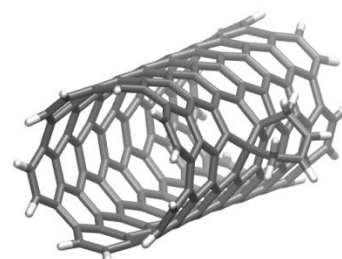
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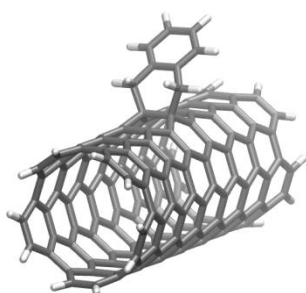
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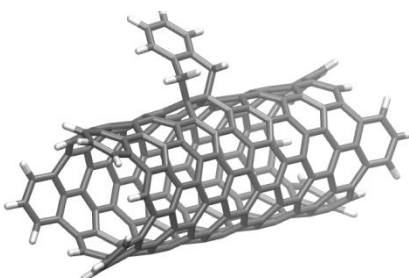
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