Supplementary information for :

Water Phase Transition Induced by a Stone-Wales Defect in a Boron Nitride Nanotube

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Details on the structure of a (5,5) SW defective BNNT are on page S1-S7, and the complete list of authors for reference 17 is listed on page S8

Nanotube structures

In this study, we considered two open-ended finite length non-defective and Stone-Wales defective (5,5) BNNTs with both ends saturated by hydrogen atoms. The tubes are approximately 26.2 Å long and 6.9 Å in diameter. We then obtained geometry optimized structures for both tubes by the AM1 semi-empirical method using Gaussian 03.[S1]

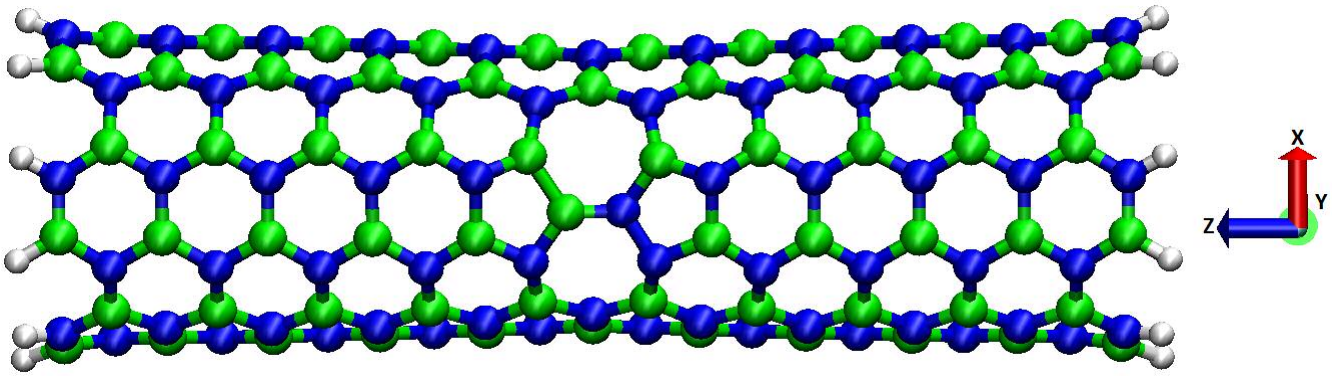

Figure S1. Optimized geometry of a SW defective (5,5) BNNT.

The optimized geometry of the BNNT is shown in Figure S1. Cartesian coordinates for the BNNT are given in the Table S1. After optimization, we obtained the AM1 energy for the SW defective BNNT to be -15.43 [hartrees].

Table S1. Cartesian coordinates of the BNNT.

	SW defective (5,5) BNNT		
Atom|Axis	X	Y	Z
B	-3.587	0.054	12.218
N	-3.267	-1.266	12.284
B	-0.950	-3.083	12.357
N	0.405	-3.212	12.376
B	2.982	-1.804	12.275
N	3.558	-0.571	12.238
B	2.809	2.257	12.150
N	1.758	3.122	12.156
B	-1.183	3.363	12.142
N	-2.381	2.716	12.167

B	-2.794	2.031	11.007
N	-3.475	0.794	11.035
B	-3.396	0.043	9.828
N	-3.133	-1.345	9.877
B	-2.711	-1.867	11.137
N	-1.666	-2.815	11.188
B	-0.974	-3.029	9.965
N	0.427	-3.220	9.967
B	1.122	-2.981	11.186
N	2.405	-2.393	11.147
B	2.783	-1.844	9.888
N	3.430	-0.586	9.828
B	3.453	0.165	11.041
N	3.200	1.553	11.006
B	2.705	2.042	9.766
N	1.660	2.996	9.751
B	0.988	3.250	10.983
N	-0.408	3.459	10.984
B	-1.073	3.182	9.758
N	-2.341	2.551	9.761
B	-2.759	1.951	8.550
N	-3.432	0.707	8.573
B	-3.378	-0.048	7.375
N	-3.146	-1.443	7.427
B	-2.688	-1.944	8.678
N	-1.668	-2.921	8.732
B	-0.978	-3.167	7.526
N	0.421	-3.378	7.535
B	1.102	-3.076	8.735
N	2.385	-2.482	8.686
B	2.775	-1.938	7.434
N	3.415	-0.676	7.377
B	3.392	0.078	8.581
N	3.159	1.473	8.546
B	2.689	1.991	7.318
N	1.675	2.980	7.310
B	0.981	3.184	8.529
N	-0.413	3.414	8.527
B	-1.089	3.154	7.312
N	-2.352	2.514	7.315
B	-2.744	1.887	6.105
N	-3.381	0.623	6.123
B	-3.324	-0.130	4.920
N	-3.107	-1.528	4.967
B	-2.685	-2.044	6.229

N	-1.675	-3.034	6.298
B	-0.986	-3.310	5.101
N	0.415	-3.535	5.117
B	1.098	-3.213	6.304
N	2.364	-2.580	6.237
B	2.729	-2.029	4.974
N	3.339	-0.754	4.920
B	3.348	-0.004	6.130
N	3.114	1.392	6.102
B	2.657	1.930	4.878
N	1.672	2.948	4.872
B	0.983	3.164	6.092
N	-0.415	3.386	6.089
B	-1.088	3.122	4.873
N	-2.337	2.454	4.873
B	-2.710	1.822	3.660
N	-3.310	0.540	3.670
B	-3.237	-0.206	2.461
N	-3.013	-1.601	2.490
B	-2.649	-2.137	3.769
N	-1.687	-3.176	3.874
B	-0.974	-3.450	2.708
N	0.425	-3.782	2.723
B	1.096	-3.387	3.889
N	2.321	-2.677	3.775
B	2.603	-2.090	2.499
N	3.216	-0.817	2.460
B	3.264	-0.076	3.677
N	3.062	1.325	3.659
B	2.627	1.891	2.440
N	1.671	2.937	2.438
B	0.981	3.148	3.656
N	-0.416	3.375	3.654
B	-1.084	3.107	2.436
N	-2.318	2.412	2.435
B	-2.674	1.781	1.218
N	-3.225	0.478	1.219
B	-3.143	-0.243	-0.001
N	-2.820	-1.623	-0.004
B	-2.498	-2.182	1.281
N	-1.537	-3.198	1.435
B	-0.400	-3.256	0.634
N	-0.368	-3.116	-0.683
B	0.898	-3.307	1.506
N	2.089	-2.667	1.277

B	2.416	-2.091	0.006
N	3.083	-0.841	0.003
B	3.161	-0.120	1.227
N	3.021	1.287	1.221
B	2.612	1.880	0.004
N	1.672	2.939	0.003
B	0.982	3.148	1.221
N	-0.415	3.378	1.219
B	-1.080	3.105	0.000
N	-2.307	2.399	-0.001
B	-2.671	1.782	-1.220
N	-3.223	0.479	-1.225
B	-3.230	-0.203	-2.466
N	-3.001	-1.601	-2.497
B	-2.482	-2.154	-1.283
N	-1.515	-3.216	-1.433
B	-1.005	-3.478	-2.741
N	0.392	-3.790	-2.742
B	0.800	-3.244	-1.506
N	2.046	-2.661	-1.258
B	2.557	-2.088	-2.486
N	3.185	-0.823	-2.450
B	3.149	-0.122	-1.218
N	3.019	1.286	-1.214
B	2.627	1.890	-2.432
N	1.675	2.940	-2.432
B	0.984	3.150	-1.215
N	-0.413	3.380	-1.216
B	-1.080	3.110	-2.435
N	-2.313	2.414	-2.437
B	-2.702	1.825	-3.662
N	-3.301	0.541	-3.675
B	-3.318	-0.127	-4.925
N	-3.112	-1.527	-4.973
B	-2.665	-2.148	-3.777
N	-1.738	-3.223	-3.890
B	-1.018	-3.332	-5.113
N	0.388	-3.536	-5.122
B	1.071	-3.385	-3.895
N	2.287	-2.673	-3.767
B	2.706	-2.031	-4.967
N	3.324	-0.760	-4.910
B	3.247	-0.083	-3.668
N	3.059	1.320	-3.651
B	2.660	1.927	-4.870

N	1.680	2.950	-4.867
B	0.988	3.152	-3.651
N	-0.409	3.379	-3.652
B	-1.079	3.126	-4.872
N	-2.327	2.457	-4.875
B	-2.733	1.891	-6.107
N	-3.372	0.627	-6.127
B	-3.375	-0.040	-7.380
N	-3.153	-1.437	-7.434
B	-2.699	-2.045	-6.238
N	-1.697	-3.045	-6.311
B	-0.994	-3.170	-7.536
N	0.406	-3.378	-7.538
B	1.077	-3.213	-6.306
N	2.343	-2.580	-6.231
B	2.763	-1.942	-7.427
N	3.408	-0.683	-7.367
B	3.341	-0.011	-6.121
N	3.117	1.387	-6.093
B	2.697	1.988	-7.311
N	1.687	2.981	-7.304
B	0.994	3.166	-6.087
N	-0.404	3.391	-6.087
B	-1.077	3.159	-7.310
N	-2.340	2.518	-7.316
B	-2.747	1.959	-8.551
N	-3.425	0.717	-8.577
B	-3.392	0.056	-9.833
N	-3.135	-1.334	-9.885
B	-2.696	-1.938	-8.687
N	-1.678	-2.917	-8.742
B	-0.980	-3.022	-9.973
N	0.421	-3.216	-9.970
B	1.092	-3.075	-8.736
N	2.376	-2.484	-8.681
B	2.781	-1.848	-9.881
N	3.433	-0.593	-9.819
B	3.394	0.072	-8.572
N	3.167	1.467	-8.537
B	2.718	2.038	-9.758
N	1.675	2.995	-9.746
B	0.996	3.186	-8.525
N	-0.398	3.417	-8.524
B	-1.057	3.187	-9.756
N	-2.326	2.559	-9.761

B	-2.781	2.043	-11.008
N	-3.467	0.809	-11.039
B	-3.582	0.072	-12.223
N	-3.265	-1.249	-12.292
B	-2.712	-1.854	-11.146
N	-1.667	-2.803	-11.197
B	-0.948	-3.069	-12.365
N	0.406	-3.202	-12.380
B	1.121	-2.977	-11.187
N	2.407	-2.395	-11.142
B	2.991	-1.808	-12.268
N	3.571	-0.578	-12.228
B	3.463	0.158	-11.031
N	3.214	1.548	-10.998
B	2.827	2.252	-12.142
N	1.778	3.120	-12.150
B	1.007	3.250	-10.979
N	-0.389	3.462	-10.982
B	-1.163	3.370	-12.140
N	-2.364	2.728	-12.167
H	-2.885	2.626	13.004
H	-3.928	0.579	13.158
H	-3.301	-1.752	13.136
H	-1.513	-3.169	13.334
H	0.880	-3.360	13.222
H	2.946	-2.358	13.259
H	3.911	-0.153	13.053
H	3.368	2.079	13.116
H	1.477	3.565	12.986
H	-0.791	3.814	13.101
H	-2.868	2.641	-13.005
H	-3.921	0.600	-13.162
H	-3.299	-1.733	-13.146
H	-1.508	-3.150	-13.344
H	0.884	-3.349	-13.225
H	2.956	-2.362	-13.252
H	3.930	-0.161	-13.041
H	3.387	2.073	-13.107
H	1.500	3.563	-12.981
H	-0.769	3.820	-13.099

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