

Supplementary Materials

In the following tables are reported the C=C and C-H interatomic distances in the different graphene nano-islands. For the hexagonal nano-islands, the central hexagon is measured as well as the six apical hexagons. For the rhombuses and triangles, one to three central hexagons are considered depending on the symmetry due to the number of hexagons on one side. We also report the interatomic distances in the four and three apical hexagons respectively. For all the geometry, the angles associated with the measured distances are listed. All the distances are given in angstrom and the angles in degree.

Table 1: C=C and C-H distances, and angles in hexagonal nano-islands

	n	2					
Central hexagon	C=C	1.4374					
	C=C	1.4374					
	C=C	1.4374					
	C=C	1.4374					
	C=C	1.4374					
	α	1.4374					
	α	120					
	α	120					
	α	120					
	α	120					
	α	120					
	α	120					
Apical hexagons	C=C	1.34876	1.34876	1.34876	1.34876	1.34876	1.34876
	C=C	1.43659	1.43659	1.43659	1.43659	1.43659	1.43659
	C=C	1.39494	1.39494	1.39494	1.39494	1.39494	1.39494
	C=C	1.4374	1.4374	1.4374	1.4374	1.4374	1.4374
	C=C	1.39494	1.39494	1.39494	1.39494	1.39494	1.39494
	C=C	1.43659	1.43659	1.43659	1.43659	1.43659	1.43659
	α	121.088	121.088	121.088	121.088	121.088	121.088
	α	121.088	121.088	121.088	121.088	121.088	121.088
	α	118.912	118.912	118.912	118.912	118.912	118.912
	α	120	120	120	120	120	120
	α	120	120	120	120	120	120
	α	118.912	118.912	118.912	118.912	118.912	118.912
	C-H	1.08277	1.08277	1.08277	1.08277	1.08277	1.08277
	C-H	1.08277	1.08277	1.08277	1.08277	1.08277	1.08277
	β	120.571	120.571	120.571	120.571	120.571	120.571
	β	118.341	118.341	118.341	118.341	118.341	118.341
	n	3					
Central hexagon	C=C	1.40897					
	C=C	1.40897					
	C=C	1.40897					
	C=C	1.40897					
	C=C	1.40897					
	α	1.40897					
	α	120					
	α	120					
	α	120					
	α	120					
	α	120					
	α	120					
Apical hexagons	C=C	1.33465	1.33465	1.33465	1.33465	1.33465	1.33465
	C=C	1.4611	1.4611	1.4611	1.4611	1.4611	1.4611
	C=C	1.4153	1.4153	1.4153	1.4153	1.4153	1.4153
	C=C	1.4446	1.4446	1.4446	1.4446	1.4446	1.4446
	C=C	1.4153	1.4153	1.4153	1.4153	1.4153	1.4153
	C=C	1.4611	1.4611	1.4611	1.4611	1.4611	1.4611
	α	121.65	121.65	121.65	121.65	121.65	121.65
	α	121.65	121.65	121.65	121.65	121.65	121.65
	α	118.157	118.157	118.157	118.157	118.157	118.157
	α	120.193	120.193	120.193	120.193	120.193	120.193
	α	120.193	120.193	120.193	120.193	120.193	120.193
	α	118.157	118.157	118.157	118.157	118.157	118.157
	C-H	1.08291	1.08291	1.08291	1.08291	1.08291	1.08291
	C-H	1.08291	1.08291	1.08291	1.08291	1.08291	1.08291
	β	120.725	120.725	120.725	120.725	120.725	120.725
	β	117.625	117.625	117.625	117.625	117.625	117.625

Table 2: C=C and C-H distances, and angles in hexagonal nano-islands - Part 2

	n	4					
Central hexagon	C=C	1.4592					
	C=C	1.41554					
	C=C	1.41554					
	C=C	1.4592					
	C=C	1.41554					
	α	1.41554					
	α	119.955					
	α	119.955					
	α	120.089					
	α	119.955					
	α	119.955					
	α	120.089					
Apical hexagons	C=C	1.3707	1.32909	1.32909	1.3707	1.32909	1.32909
	C=C	1.417	1.46689	1.47415	1.417	1.46689	1.47415
	C=C	1.41118	1.44419	1.44872	1.41118	1.44419	1.44872
	C=C	1.42566	1.40805	1.40805	1.42566	1.40805	1.40805
	C=C	1.41118	1.44872	1.44419	1.41118	1.44872	1.44419
	C=C	1.417	1.47415	1.46689	1.417	1.47415	1.46689
	α	121.412	122.06	122.172	121.412	122.06	122.172
	α	121.412	122.172	122.06	121.412	122.172	122.06
	α	118.331	117.18	116.835	118.331	117.18	116.835
	α	120.256	120.878	120.875	120.256	120.878	120.875
	α	120.256	120.875	120.878	120.256	120.875	120.878
	α	118.331	116.835	117.18	118.331	116.835	117.18
	C-H	1.08335	1.08239	1.08349	1.08335	1.08239	1.08349
	C-H	1.08335	1.08349	1.08239	1.08335	1.08349	1.08239
	β	119.836	120.806	120.538	119.836	120.806	120.538
	β	118.751	117.29	117.133	118.751	117.29	117.133
	n	5					
Central hexagon	C=C	1.41169					
	C=C	1.41169					
	C=C	1.41169					
	C=C	1.41169					
	C=C	1.41169					
	α	1.41169					
	α	120					
	α	120					
	α	120					
	α	120					
	α	120					
	α	120					
Apical hexagons	C=C	1.32594	1.32594	1.32594	1.32594	1.32594	1.32594
	C=C	1.47766	1.47766	1.47766	1.47766	1.47766	1.47766
	C=C	1.45612	1.45612	1.45612	1.45612	1.45612	1.45612
	C=C	1.41531	1.41531	1.41531	1.41531	1.41531	1.41531
	C=C	1.45612	1.45612	1.45612	1.45612	1.45612	1.45612
	C=C	1.47766	1.47766	1.47766	1.47766	1.47766	1.47766
	α	122.191	122.191	122.191	122.191	122.191	122.191
	α	122.191	122.191	122.191	122.191	122.191	122.191
	α	117.149	117.149	117.149	117.149	117.149	117.149
	α	120.66	120.66	120.66	120.66	120.66	120.66
	α	120.66	120.66	120.66	120.66	120.66	120.66
	α	117.149	117.149	117.149	117.149	117.149	117.149
	C-H	1.08307	1.08307	1.08307	1.08307	1.08307	1.08307
	C-H	1.08307	1.08307	1.08307	1.08307	1.08307	1.08307
	β	120.761	120.761	120.761	120.761	120.761	120.761
	β	117.048	117.048	117.048	117.048	117.048	117.048

Table 3: C=C and C-H distances, and angles in hexagonal nano-islands - Part 3

	n	6					
Central hexagon	C=C	1.44322					
	C=C	1.44159					
	C=C	1.44159					
	C=C	1.44322					
	C=C	1.44159					
	α	1.44159					
	α	120.035					
	α	120.035					
	α	119.929					
	α	120.035					
	α	120.035					
	α	119.929					
Apical hexagons	C=C	1.3318	1.33092	1.33092	1.3318	1.33092	1.33092
	C=C	1.45921	1.47967	1.47599	1.45921	1.47967	1.47599
	C=C	1.42537	1.42843	1.48701	1.42537	1.42843	1.48701
	C=C	1.41741	1.40408	1.40408	1.41741	1.40408	1.40408
	C=C	1.42537	1.48701	1.42843	1.42537	1.48701	1.42843
	C=C	1.45921	1.47599	1.47967	1.45921	1.47599	1.47967
	α	122.646	122.971	123.786	122.646	122.971	123.786
	α	122.646	123.786	122.971	122.646	123.786	122.971
	α	115.873	116.664	112.235	115.873	116.664	112.235
	α	121.481	119.02	125.324	121.481	119.02	125.324
	α	121.481	125.324	119.02	121.481	125.324	119.02
	α	115.873	112.235	116.664	115.873	112.235	116.664
	C-H	1.08364	1.08301	1.08395	1.08364	1.08301	1.08395
	C-H	1.08364	1.08395	1.08301	1.08364	1.08395	1.08301
	β	120.914	120.825	119.493	120.914	120.825	119.493
	β	116.441	116.721	116.204	116.441	116.721	116.204

Table 4: C=C and C-H distances, and angles in rhombus nano-islands

	n	2				4			
Central hexagons	C=C					1.43849		1.39962	
	C=C					1.38935		1.43299	
	C=C					1.43849		1.39962	
	C=C					1.39962		1.43849	
	C=C					1.43299		1.38935	
	C=C					1.39962		1.43849	
	α					120.002		120.002	
	α					120.055		119.943	
	α					120.055		119.943	
	α					120.002		120.002	
	α					119.943		120.055	
	α					119.943		120.055	
Apical hexagons	C=C	1.3853	1.46214	1.3853	1.46214	1.37864	1.47243	1.37864	1.47243
	C=C	1.39453	1.33275	1.39453	1.33275	1.45968	1.32834	1.45968	1.32834
	C=C	1.41302	1.46214	1.41302	1.46214	1.44154	1.47243	1.44154	1.47243
	C=C	1.41302	1.41302	1.41302	1.41302	1.44154	1.43778	1.44154	1.43778
	C=C	1.39453	1.44592	1.39453	1.44592	1.45968	1.43299	1.45968	1.43299
	C=C	1.3853	1.41302	1.3853	1.41302	1.37864	1.43778	1.37864	1.43778
	α	120.531	118.511	120.531	118.511	121.501	117.669	121.501	117.669
	α	120.583	121.475	120.583	121.475	121.122	121.957	121.122	121.957
	α	119.167	121.475	119.167	121.475	117.97	121.957	117.97	121.957
	α	119.97	118.511	119.97	118.511	120.315	117.669	120.315	117.669
	α	119.167	120.015	119.167	120.015	117.97	120.374	117.97	120.374
	α	120.583	120.015	120.583	120.015	121.122	120.374	121.122	120.374
	C-H	1.08267	1.08287	1.08267	1.08287	1.08295	1.083	1.08295	1.083
	C-H	1.08254	1.08287	1.08254	1.08287	1.08227	1.083	1.08227	1.083
	C-H	1.08254		1.08254		1.08227		1.08227	
	β	119.735	120.899	119.735	120.899	119.25	120.798	119.25	120.798
	β	119.412	117.626	119.412	117.626	118.296	117.244	118.296	117.244
	β	120.006	-	120.006		120.582		120.582	

Table 5: C=C and C-H distances, and angles in rhombus nano-islands - Part 2

	n	5				6			
Central hexagons	C=C	1.40965				1.41246		1.44194	
	C=C	1.40916				1.43576		1.39775	
	C=C	1.40965				1.41246		1.44194	
	C=C	1.40965				1.44194		1.41246	
	C=C	1.40916				1.39775		1.43576	
	C=C	1.40965				1.44194		1.41246	
	α	119.848				119.798		119.798	
	α	120.076				120.003		120.199	
	α	120.076				120.003		120.199	
	α	119.848				119.798		119.798	
	α	120.076				120.199		120.003	
	α	120.076				120.199		120.003	
Apical hexagons	C=C	1.38363	1.46205	1.38363	1.46205	1.38357	1.47657	1.38357	1.47657
	C=C	1.39847	1.33379	1.39847	1.33379	1.3985	1.32615	1.3985	1.32615
	C=C	1.40844	1.46205	1.40844	1.46205	1.40845	1.47657	1.40845	1.47657
	C=C	1.40844	1.41718	1.40844	1.41718	1.40845	1.45262	1.40845	1.45262
	C=C	1.39847	1.4432	1.39847	1.4432	1.3985	1.4179	1.3985	1.4179
	C=C	1.38363	1.41718	1.38363	1.41718	1.38357	1.45262	1.38357	1.45262
	α	120.097	118.181	120.097	118.181	120.081	117.32	120.081	117.32
	α	120.668	121.644	120.668	121.644	120.673	122.105	120.673	122.105
	α	119.561	121.644	119.561	121.644	119.582	122.105	119.582	122.105
	α	119.446	118.181	119.446	118.181	119.409	117.32	119.409	117.32
	α	119.561	120.175	119.561	120.175	119.582	120.574	119.582	120.574
	α	120.668	120.175	120.668	120.175	120.673	120.574	120.673	120.574
	C-H	1.08264	1.0829	1.08264	1.0829	1.08264	1.08305	1.08264	1.08305
	C-H	1.08228	1.0829	1.08228	1.0829	1.08228	1.08305	1.08228	1.08305
	C-H	1.08228		1.08228		1.08228		1.08228	
	β	119.952	120.766	119.952	120.766	119.959	120.805	119.959	120.805
	β	119.198	117.59	119.198	117.59	119.189	117.089	119.189	117.089
	β	120.134		120.134		120.138		120.138	

Table 6: C=C and C-H distances, and angles in rhombus nano-islands - Part 3

	n	7			
Central hexagons	C=C	1.43439			
	C=C	1.43215			
	C=C	1.43439			
	C=C	1.43439			
	C=C	1.43215			
	C=C	1.43439			
	α	119.666			
	α	120.167			
	α	120.167			
	α	119.666			
	α	120.167			
	α	120.167			
Apical hexagons	C=C	1.37931	1.47014	1.37931	1.47014
	C=C	1.44628	1.32848	1.44628	1.32848
	C=C	1.43752	1.47014	1.43752	1.47014
	C=C	1.43752	1.43381	1.43752	1.43381
	C=C	1.44628	1.43632	1.44628	1.43632
	C=C	1.37931	1.43381	1.37931	1.43381
	α	121.305	118.039	121.305	118.039
	α	121.058	121.791	121.058	121.791
	α	118.246	121.791	118.246	121.791
	α	120.087	118.039	120.087	118.039
	α	118.246	120.17	118.246	120.17
	α	121.058	120.17	121.058	120.17
	C-H	1.0829	1.08292	1.0829	1.08292
	C-H	1.08231	1.08292	1.08231	1.08292
	C-H	1.08231		1.08231	
	β	119.348	120.904	119.348	120.904
	β	118.414	117.306	118.414	117.306
	β	120.528		120.528	

Table 7: C=C and C-H distances, and angles in triangle nano-islands

	n	2			3			4		
Central hexagons	C=C							1.41058		
	C=C							1.41058		
	C=C							1.41058		
	C=C							1.41058		
	C=C							1.41058		
	C=C							1.41058		
	α							119.88		
	α							120.12		
	α							119.88		
	α							120.12		
Apical hexagons	C=C	1.38245	1.38245	1.38245	1.38215	1.38215	1.38215	1.38372	1.38372	1.38372
	C=C	1.41576	1.41576	1.41576	1.41815	1.41815	1.41815	1.40279	1.40279	1.40279
	C=C	1.42545	1.42545	1.42545	1.42819	1.42819	1.42819	1.4161	1.4161	1.4161
	C=C	1.42545	1.42545	1.42545	1.42819	1.42819	1.42819	1.4161	1.4161	1.4161
	C=C	1.41576	1.41576	1.41576	1.41815	1.41815	1.41815	1.40279	1.40279	1.40279
	C=C	1.38245	1.38245	1.38245	1.38215	1.38215	1.38215	1.38372	1.38372	1.38372
	α	120.928	120.928	120.928	120.981	120.981	120.981	120.544	120.544	120.544
	α	120.818	120.818	120.818	120.895	120.895	120.895	120.711	120.711	120.711
	α	118.718	118.718	118.718	118.589	118.589	118.589	119.075	119.075	119.075
	α	120	120	120	120.049	120.049	120.049	119.885	119.885	119.885
	α	118.718	118.718	118.718	118.589	118.589	118.589	119.075	119.075	119.075
	α	120.818	120.818	120.818	120.895	120.895	120.895	120.711	120.711	120.711
	C-H	1.08278	1.08278	1.08278	1.08278	1.08278	1.08278	1.08269	1.08269	1.08269
	C-H	1.08242	1.08242	1.08242	1.08237	1.08237	1.08237	1.08238	1.08238	1.08238
	C-H	1.08242	1.08242	1.08242	1.08237	1.08237	1.08237	1.08238	1.08238	1.08238
	β	119.536	119.536	119.536	119.509	119.509	119.509	119.728	119.728	119.728
	β	118.968	118.968	118.968	118.883	118.883	118.883	119.174	119.174	119.174
	β	120.214	120.214	120.214	120.221	120.221	120.221	120.115	120.115	120.115

Table 8: C=C and C-H distances, and angles in triangle nano-islands - Part2

	n	5			6			7		
Central hexagons	C=C	1.41308	1.42345	1.42596	1.42446	1.41999	1.42167	1.41189		
	C=C	1.42345	1.41308	1.42596	1.42167	1.41999	1.42446	1.41189		
	C=C	1.42596	1.41308	1.42345	1.42167	1.42446	1.41999	1.41189		
	C=C	1.42596	1.42345	1.41308	1.42446	1.42617	1.41999	1.41189		
	C=C	1.42345	1.42596	1.41308	1.41999	1.42617	1.42446	1.41189		
	C=C	1.41308	1.42596	1.42345	1.41999	1.42446	1.42167	1.41189		
	α	120.31	119.628	119.628	119.894	119.894	120	119.822		
	α	120.217	120.217	120	119.996	120.22	119.996	120.178		
	α	119.628	120.31	119.628	120	119.894	119.894	119.822		
	α	120	120.217	120.217	119.996	119.996	120.22	120.178		
	α	119.628	119.628	120.31	119.894	120	119.894	119.822		
	α	120.217	120	120.217	120.22	119.996	119.996	120.178		
Apical hexagons	C=C	1.38396	1.38396	1.38396	1.3833	1.3833	1.3833	1.38438	1.38438	1.38438
	C=C	1.40091	1.40091	1.40091	1.40786	1.40786	1.40786	1.39841	1.39841	1.39841
	C=C	1.4169	1.4169	1.4169	1.42268	1.42268	1.42268	1.41454	1.41454	1.41454
	C=C	1.4169	1.4169	1.4169	1.42268	1.42268	1.42268	1.41454	1.41454	1.41454
	C=C	1.40091	1.40091	1.40091	1.40786	1.40786	1.40786	1.39841	1.39841	1.39841
	C=C	1.38396	1.38396	1.38396	1.3833	1.3833	1.3833	1.38438	1.38438	1.38438
	α	120.554	120.554	120.554	120.768	120.768	120.768	120.522	120.522	120.522
	α	120.675	120.675	120.675	120.79	120.79	120.79	120.621	120.621	120.621
	α	119.203	119.203	119.203	118.878	118.878	118.878	119.237	119.237	119.237
	α	119.69	119.69	119.69	119.897	119.897	119.897	119.763	119.763	119.763
	α	119.203	119.203	119.203	118.878	118.878	118.878	119.237	119.237	119.237
	α	120.675	120.675	120.675	120.79	120.79	120.79	120.621	120.621	120.621
	C-H	1.08273	1.08273	1.08273	1.08274	1.08274	1.08274	1.08274	1.08274	1.08274
	C-H	1.08237	1.08237	1.08237	1.0824	1.0824	1.0824	1.08237	1.08237	1.08237
	C-H	1.08237	1.08237	1.08237	1.0824	1.0824	1.0824	1.08237	1.08237	1.08237
	β	119.723	119.723	119.723	119.616	119.616	119.616	119.739	119.739	119.739
	β	119.208	119.208	119.208	119.072	119.072	119.072	119.284	119.284	119.284
	β	120.117	120.117	120.117	120.138	120.138	120.138	120.095	120.095	120.095

Table 9: Basis set effects for the smallest edifices (energies in hartree at the STO-3G optimized geometry)

	STO-3G	ANO _{VDZ}	ANO _{VTZ}	ANO _{VQZ}
H_2	-904.822707	-916.150544	-916.262871	-916.275288
	-905.074409	-916.513558	-916.660075	-916.683710
R_3	-1129.094416	-1143.502335	-1143.637361	-1143.654838
	-1129.412242	-1143.940113	-1144.119948	-
T_3	-829.887993	-840.301482	-840.404356	-840.415641
	-830.135220	-840.649106	-840.782867	-840.804340

ANO_{VDZ}: (3s3p1d) / ANO_{VTZ}: (4s3p2d1f) / ANO_{VQZ}: (5s4p3d2f)

Table 10: Active space size effect on NEVPT2 energies (in hartree)

	Min.	Min. + 2 orbitals	Min. + 4 orbitals
R_4	-1806.692777	-1806.692039	-1806.688307
T_3	-830.135221	-830.135218	-830.129385