Electronic Supplementary Material (ESI) for Nanoscale.

SUPPLEMENTARY INFORMATION

Boron Doping of Graphene – Pushing the Limit

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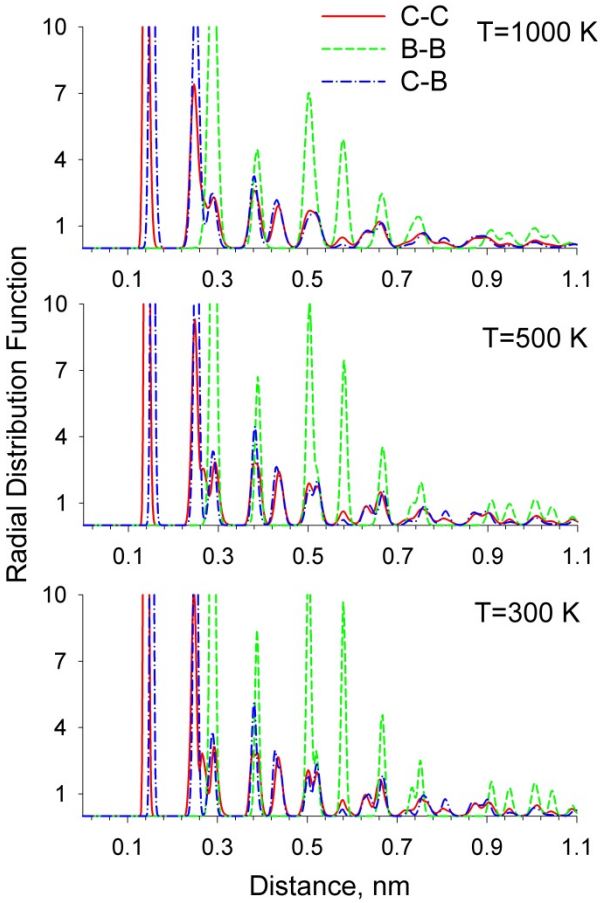

Figure S1. Radial distribution functions for carbon-carbon (red solid line), boron-boron (green dashed line), and carbon-boron (blue dash-dotted line) distances computed from the 100 ps long trajectory for the “para” system.

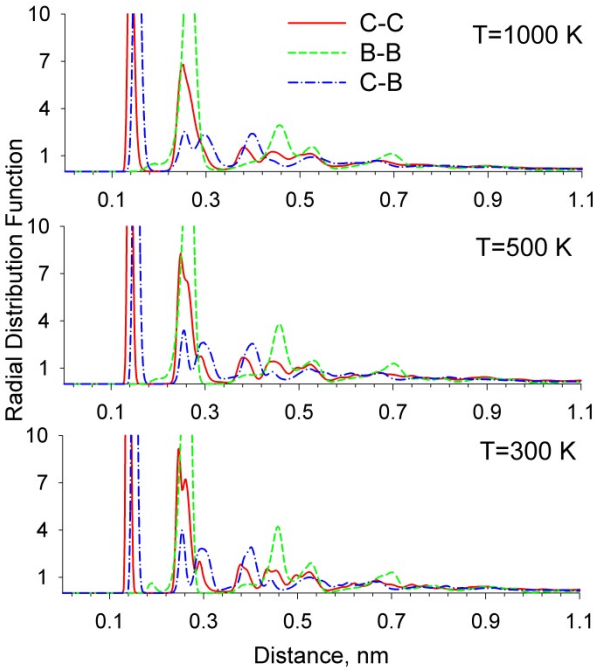

Figure S2. Radial distribution functions for carbon-carbon (red solid line), boron-boron (green dashed line), and carbon-boron (blue dash-dotted line) distances computed from the 100 ps long trajectory for the “meta” system.

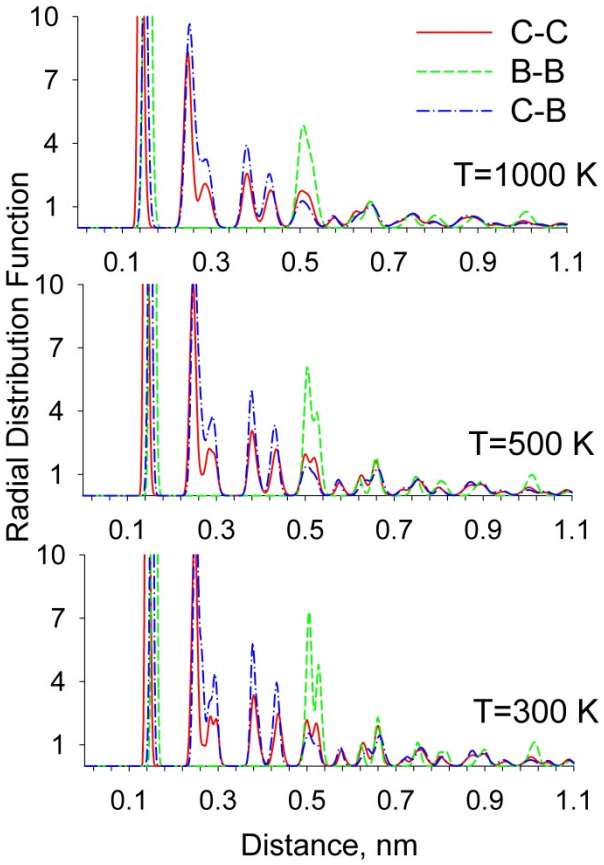

Figure S3. Radial distribution functions for carbon-carbon (red solid line), boron-boron (green dashed line), and carbon-boron (blue dash-dotted line) distances computed from the 100 ps long trajectory for the “B-B” system.

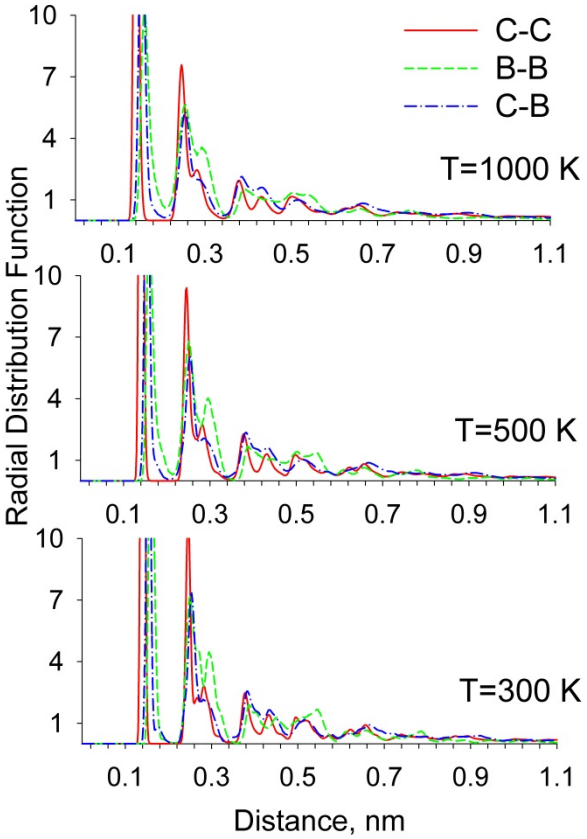

Figure S4. Radial distribution functions for carbon-carbon (red solid line), boron-boron (green dashed line), and carbon-boron (blue dash-dotted line) distances computed from the 100 ps long trajectory for the “3B” system.

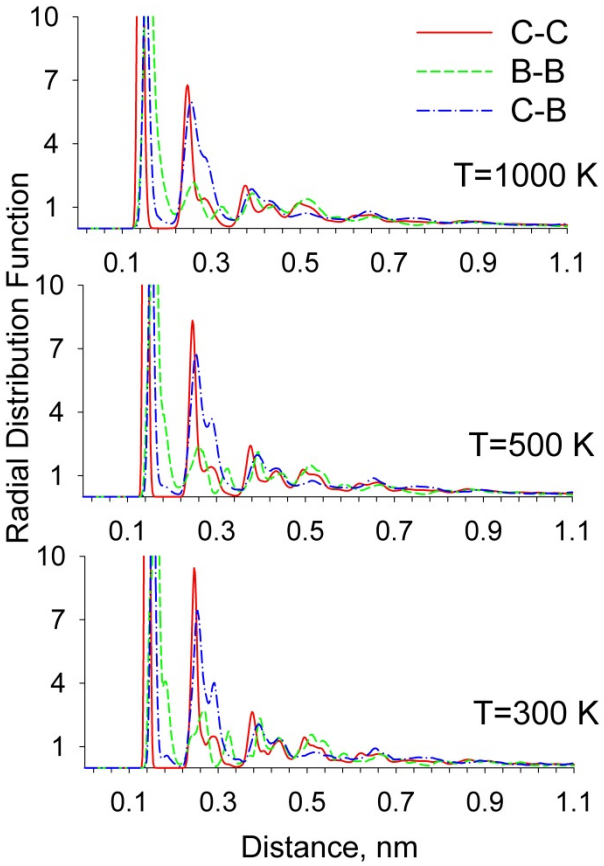

Figure S5. Radial distribution functions for carbon-carbon (red solid line), boron-boron (green dashed line), and carbon-boron (blue dash-dotted line) distances computed from the 100 ps long trajectory for the “B-B-B” system.

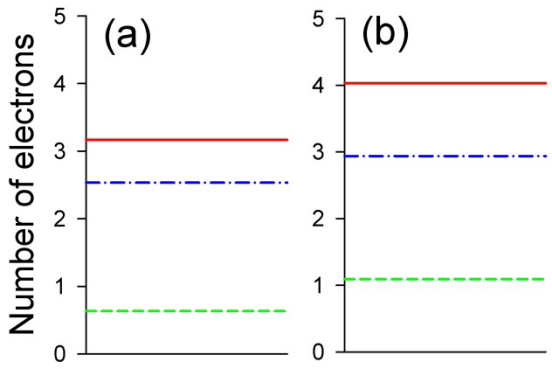

Figure S6. Total number of electrons localized on (a) boron and (b) carbon atoms (red solid line). Populations of 2s (green dashed line) and 2p (blue dash-dotted line) orbitals. The boron atoms have less than one 2s-electron and 2.5 2p-electrons, whereas the carbon atoms have one 2s-electron and three 2p-electrons. The excessive electron density on boron arrives from hydrogen atoms through carbon atoms. The data were averaged over all carbon and all boron atoms in the “1B” and “meta” systems in their optimized geometries. The averages computed separately for “1B” and “meta” are identical.

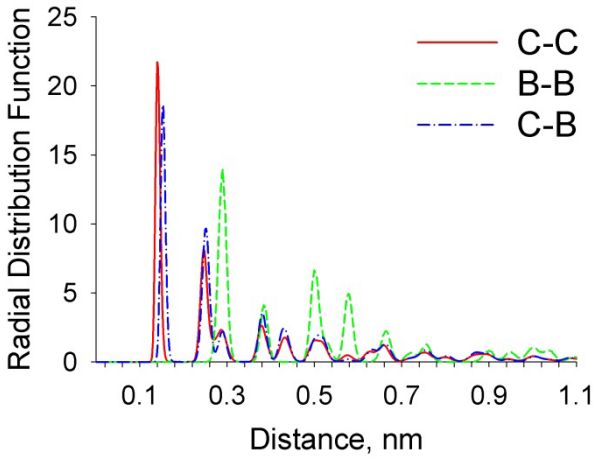

Figure S7. Radial distribution functions for carbon-carbon (red solid line), boron-boron (green dashed line), and carbon-boron (blue dash-dotted line) distances computed from the 100 ps long trajectory for the “big” system.

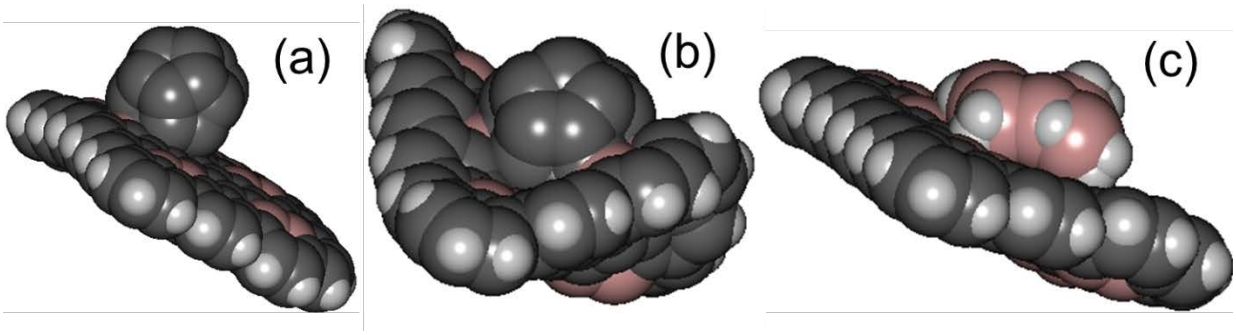

Figure S8. Molecular configurations obtained from PM7-MD simulations of the “B-B” B-doped graphene in contact with C_{20} (a, b) and decaborane $B_{10}H_{14}$ (c).

Table S1. Most probable covalent and non-covalent carbon-carbon, boron-boron, and carbon-boron distances and RDF peaks in the B-doped graphene for the “para” and “big” systems (see Table 1). R_1-R_4 are the positions of the first four peaks, whereas h_1-h_4 are the dimensionless heights of the first four peaks

	C-C		B-B		C-B	
system	“para”	“big”	“para”	“big”	“para”	“big”
R_1, Å	1.40	1.40	2.90	2.90	1.54	1.54
h_1	22.3	21.7	14.8	14.0	22.7	18.6
R_2, Å	2.48	2.46	3.88	3.84	2.52	2.52
h_2	7.4	8.2	4.5	4.1	12.0	9.7
R_3, Å	2.92	2.86	5.04	5.00	3.82	2.90
h_3	2.3	2.3	7.0	6.6	3.3	2.2
R_4, Å	3.82	3.78	5.78	5.78	4.32	3.80
h_4	2.6	2.6	4.9	4.9	2.2	3.5