

Quantum Chemical Molecular Dynamics Simulations of Dynamic Fullerene Self-Assembly in Benzene Combustion [*ACS Nano* 2009, 3, 2241–2257].

Biswajit Saha, Sho Shindo, Stephan Irle,* and Keiji Morokuma*

The rms values for curvature given in the last column of Table 2, Table 4, and Table 6 were incorrect. The curvature values should read as given below.

TABLE 2. List of Successful Simulations with $T_n = 2500$ K

trajectory name	curvature (1/Å)
B2500Kg1_4	0.228
B2500Kg1_5	0.234
B2500Kg1_7	0.217
B2500Kg1_8	0.231
B2500Kg1_11	0.221
B2500Kg1_12	0.224
B2500Kg1_14	0.219
B2500Kg1_16	0.220
B2500Kg1_18	0.234
B2500Kg1_19	0.210

TABLE 4. Successful Simulations with $T_n = 3000$ K

trajectory name	curvature (1/Å)
B3000Kg1_1	0.232
B3000Kg1_2	0.243
B3000Kg1_3	0.225
B3000Kg1_4	0.242
B3000Kg1_13	0.230
B3000Kg1_15	0.232
B3000Kg2_2	0.218
B3000Kg2_3	0.220
B3000Kg2_5	0.235
B3000Kg2_6	0.240
B3000Kg2_7	0.238
B3000Kg2_10	0.232
B3000Kg2_12	0.218
B3000Kg2_13	0.229
B3000Kg3_3	0.232
B3000Kg3_4	0.237
B3000Kg3_7	0.263
B3000Kg3_8	0.228
B3000Kg3_13	0.257
B3000Kg3_14	0.220
B3000Kg4_3	0.234
B3000Kg4_6	0.264
B3000Kg4_7	0.210
B3000Kg4_9	0.209
B3000Kg4_10	0.234

TABLE 6. List of Successful Simulations Using SCC-DFTB (Followed by NCC-DFTB) with $T_n = 2500$ K, $T_e = 2500$ K

trajectory name	curvature (1/Å)
BSN2500Kg1_1	0.214
BSN2500Kg1_2	0.236
BSN2500Kg1_6	0.209
BSN2500Kg1_7	0.227

Correspondingly, we make two corrections in the text as follows.

Text change 1:

Page 2246 column 2, middle paragraph:

“The average cage sizes and corresponding rms curvatures of the giant fullerenes at $T_n = 2500$ K are 191.9 and 0.136 \AA^{-1} , and at $T_n = 3000$ K they are 160.7 and 0.143 \AA^{-1} .” should read:

“The average cage sizes and corresponding rms curvatures of the giant fullerenes at $T_n = 2500$ K are 191.9 and 0.224 \AA^{-1} , and at $T_n = 3000$ K they are 160.7 and 0.233 \AA^{-1} .”

Text change 2:

Page 2246 column 2, last paragraph:

“As in our previous simulations of pure carbon systems, the average rms curvatures of self-assembled GFs are higher than one would expect for spherical cages, but much lower than the curvature required for $^{1h}C_{60}$, which has an rms curvature of 0.28 \AA^{-1} . If the cages were spherical, a 0.13 \AA^{-1} rms curvature would correspond to a radius of 7.69 \AA and therefore contain more than 240 atoms (the radius of $^{1h}C_{240}$ is $\sim 7.3 \text{ \AA}$). Generally, the cages emerge with very nonspherical shape and therefore larger local curvature values are observed.”

should read:

“As in our previous simulations of pure carbon systems, the average rms curvatures of self-assembled GFs are much higher than one would expect for spherical cages of this size, but lower than the curvature required for $^{1h}C_{60}$, which has a rms curvature of 0.28 \AA^{-1} . If the cages were spherical, a 0.22 \AA^{-1} rms curvature would correspond to a radius of 4.55 \AA and therefore contain ~ 80 atoms (the radius of $^{1h}C_{80}$ is $\sim 4.07 \text{ \AA}$). Generally, the cages emerge with very nonspherical shape and therefore larger local curvature values are observed.”

The changes do not affect the reported trajectories and conclusions of the paper.

Published online December 10, 2009.
10.1021/nn901665j