# Supporting Information

## Extraordinary Improvement of Graphitic Structure of Continuous Carbon Nanofibers Templated with Double Wall Carbon Nanotubes

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**1. MD Simulation of Evolution of Small Molecular Species during Templated Carbonization**

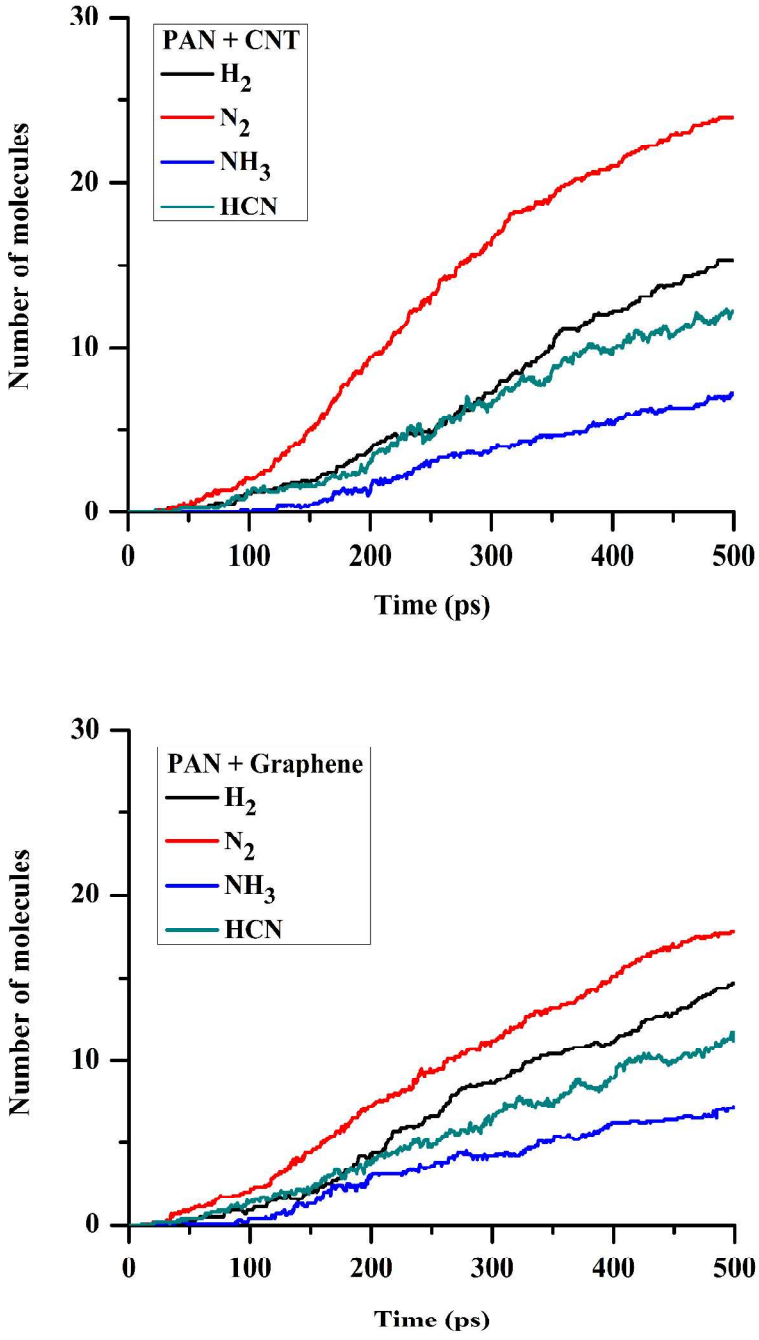



Figure S1. Number of small molecular species formed during simulations at 2500K and with density 1.6 gm/cc. Averaged over 10 trajectories.

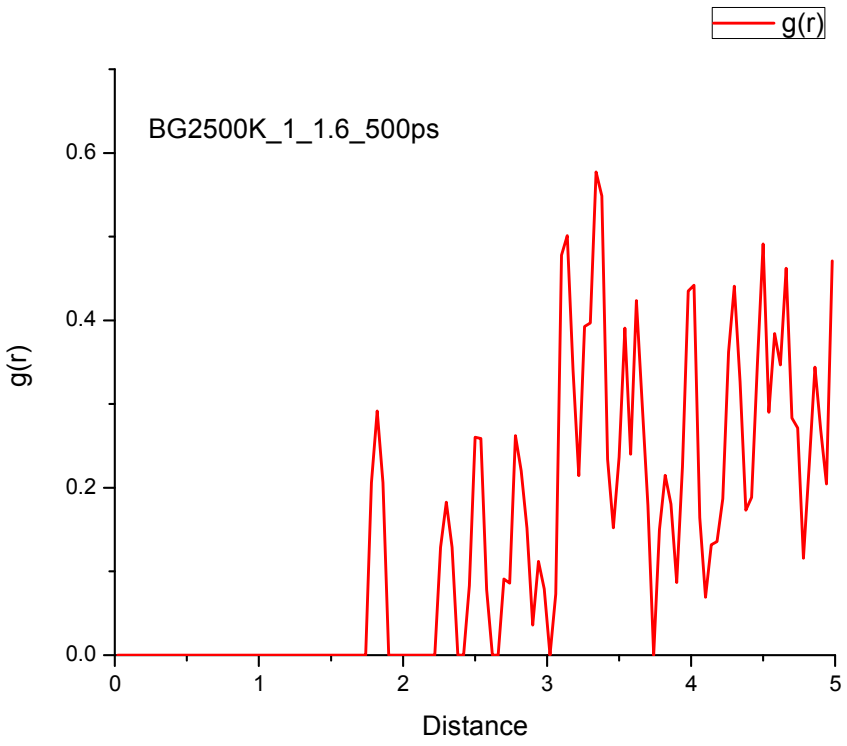
Table S1 Species evolution rate (number of molecules/ns) for simulations at 2500K and density 1.6 gm/cc. Averaged over 10 trajectories.

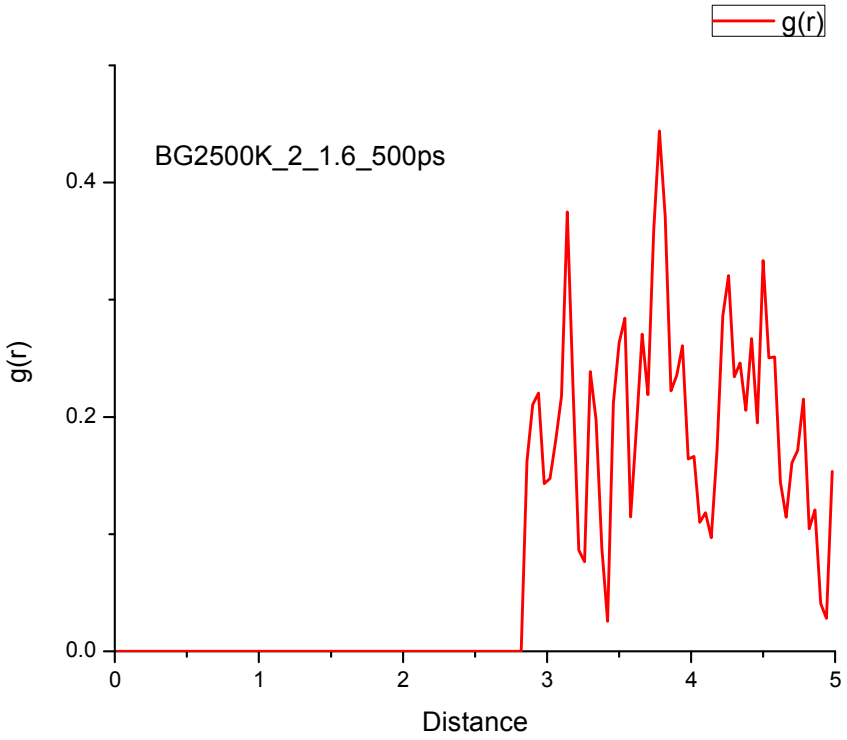
| Model | $H_2$ | $N_2$ | $NH_3$ | HCN |
|---|---|---|---|---|
| PAN | 30.1 | 51.5 | 20.3 | 21.8 |
| PAN + CNT | 30.7 | 47.8 | 14.4 | 24.4 |
| PAN + Graphene | 30.0 | 35.8 | 12.9 | 23.1 |

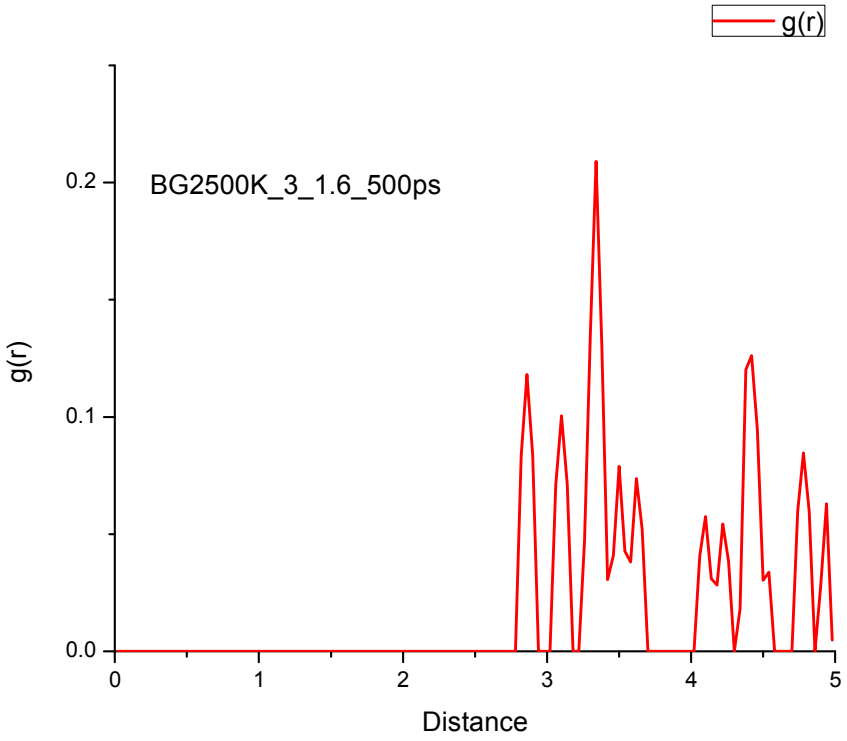
**2. Radial distribution functions as a function of the distance from the graphene or CNT and carbon atoms that are in the pure carbon-containing rings**

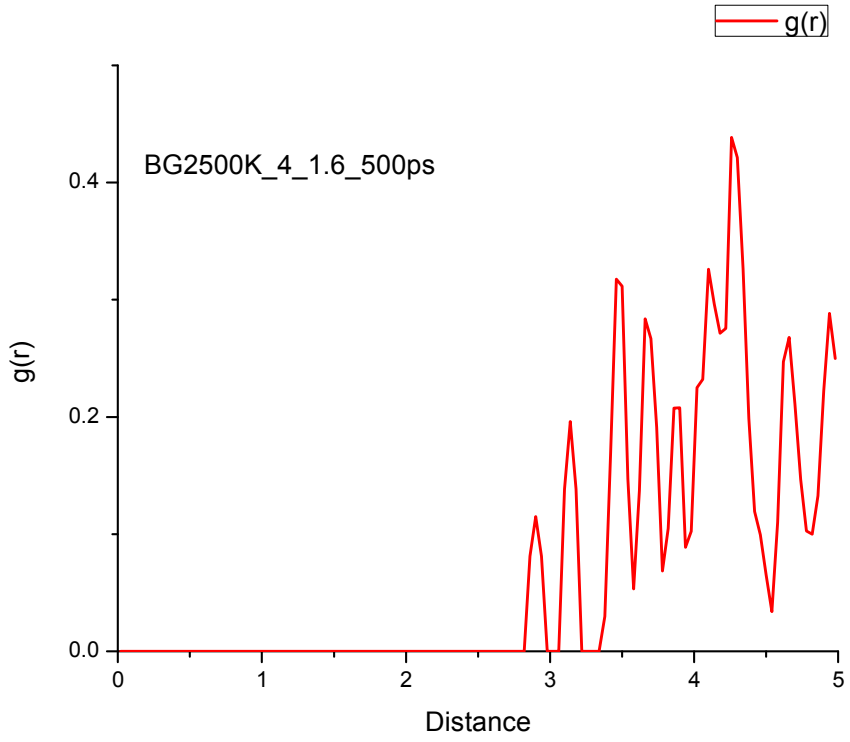
The first five plots below present the radial distribution function, g(r), associated with C-atoms on the graphene sheet and C-atoms on the newly formed carbon ring structures. The five plots refer to different independent molecular dynamics simulations, all at 2500K. It is apparent from these plots that the separation between the graphene sheet and newly formed structure generally varies between ~3.0 to 3.5 Å, which is a typically graphene-graphene distance. Only in case of BG2500K_1 is there bond formation, leading to a nonzero g(r) below 2.5 Å.

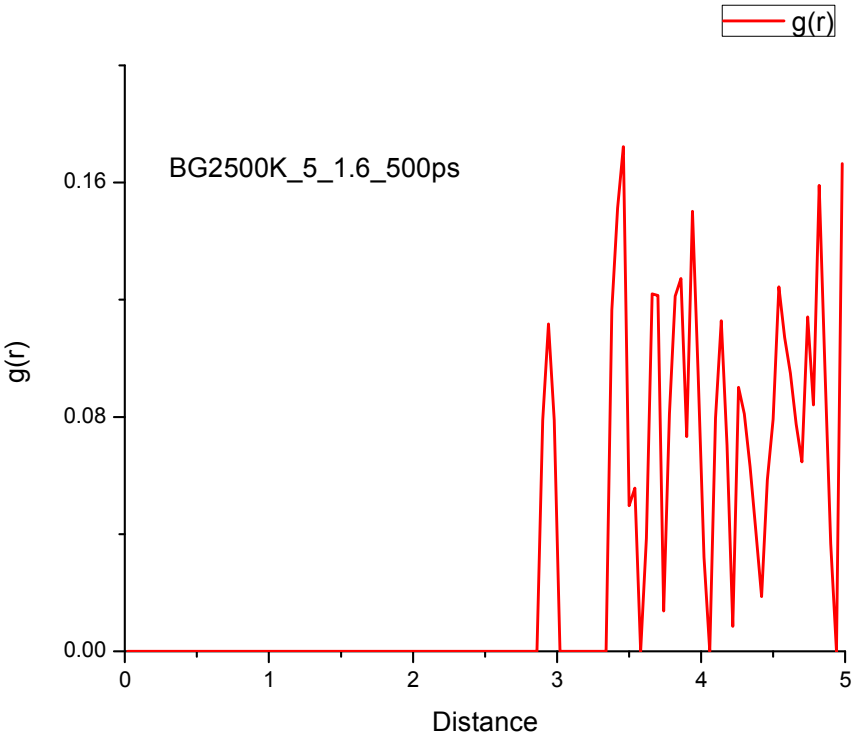
The remaining plots refer to similar g(r) plots for PAN+CNT simulations at 2500K with the first three showing results for a density of 1.6 and the rest for a density of 1.74. The results show that for simulation times up to 500 ps there is no structure is formed with some preferred alignment.

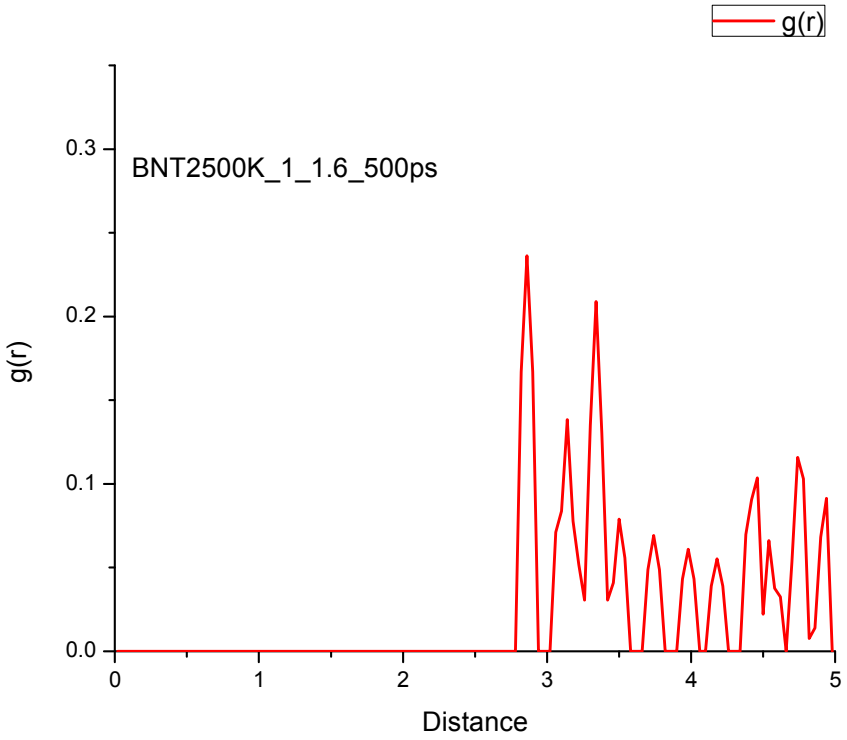

g(r)
BG2500K_1_1.6_500ps
0.6
0.4
0.2
0.0
g(r)
0
1
2
3
4
5
Distance

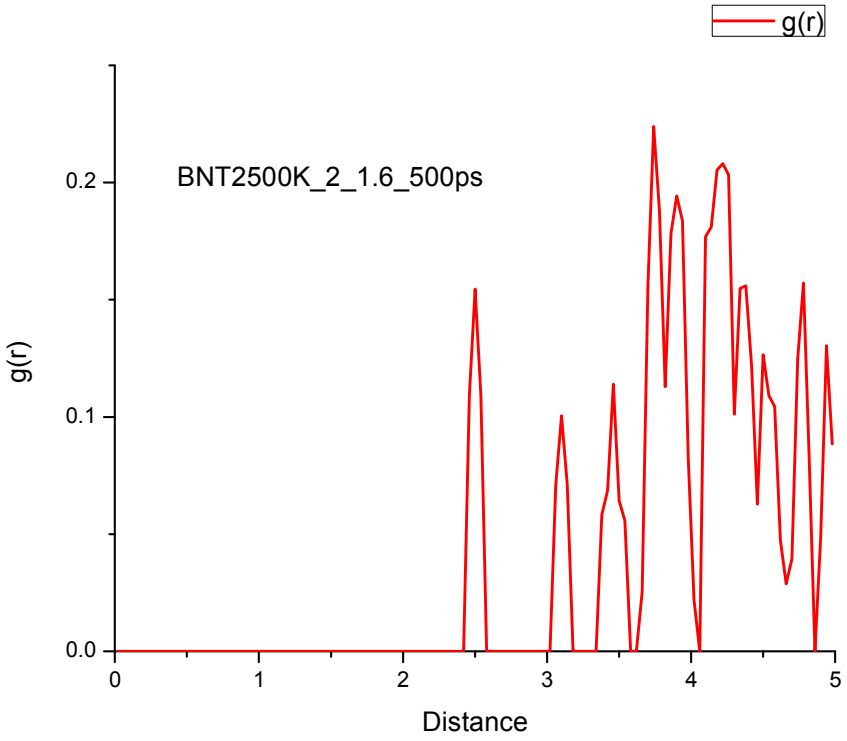

g(r)
BG2500K_2_1.6_500ps
0.4
0.2
0.0
g(r)
0
1
2
3
4
5
Distance

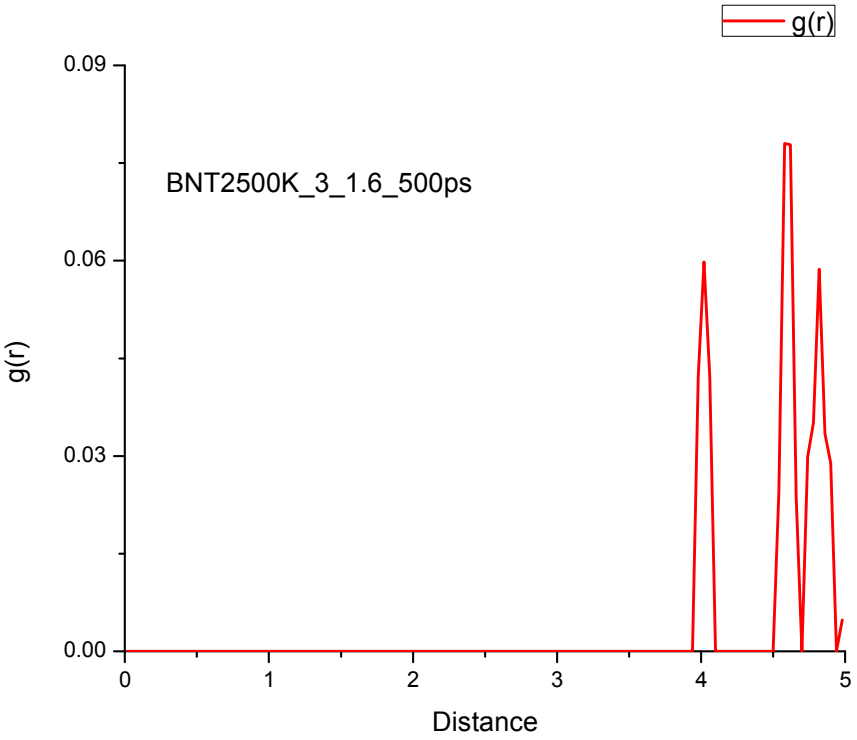

g(r)
BG2500K_3_1.6_500ps
0.2
0.1
0.0
g(r)
0
1
2
3
4
5
Distance

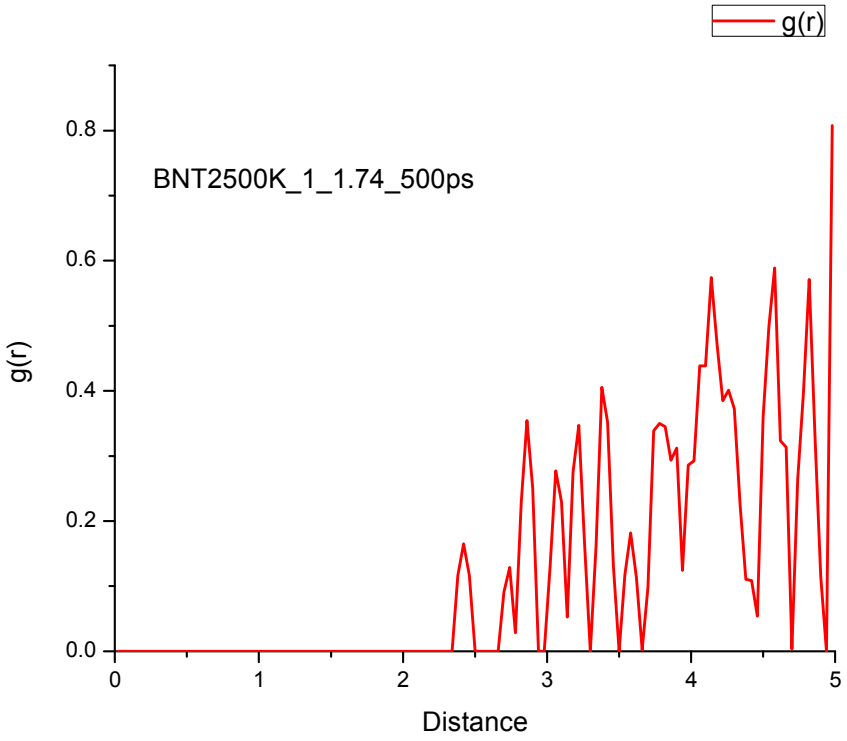

g(r)
BG2500K_4_1.6_500ps
g(r)
0.0
0.2
0.4
0
1
2
3
4
5
Distance

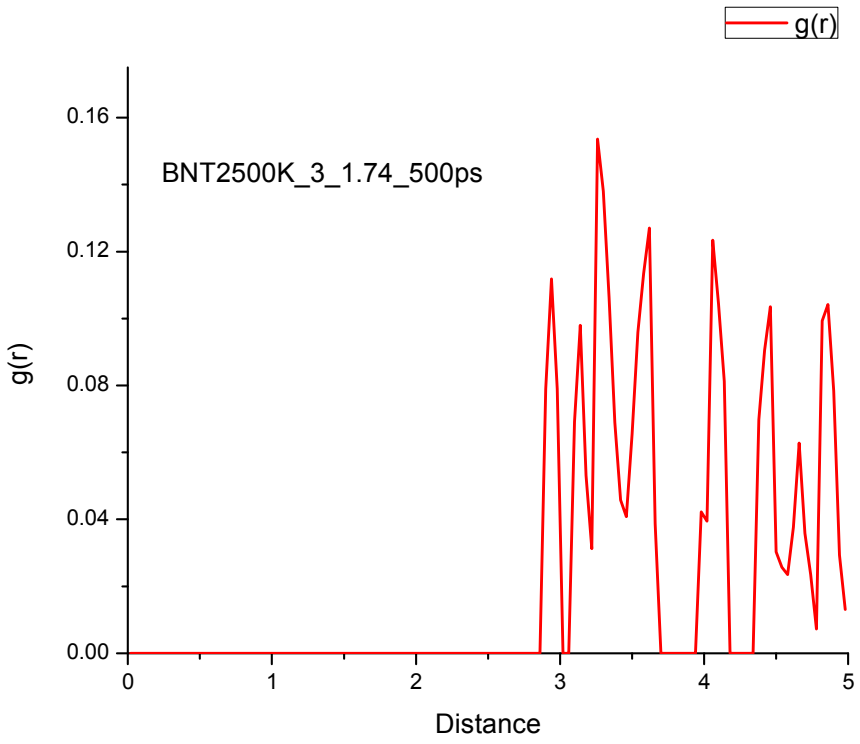

g(r)
BG2500K_5_1.6_500ps
g(r)
0.00
0.08
0.16
0
1
2
3
4
5
Distance


g(r)
BNT2500K_1_1.6_500ps
g(r)
0.0
0.1
0.2
0.3
0
1
2
3
4
5
Distance


g(r)
BNT2500K_2_1.6_500ps
g(r)
0.0
0.1
0.2
0
1
2
3
4
5
Distance


g(r)
BNT2500K_3_1.6_500ps
0.09
0.06
0.03
0.00
g(r)
0
1
2
3
4
5
Distance


g(r)
BNT2500K_1_1.74_500ps
0.8
0.6
0.4
0.2
0.0
g(r)
0
1
2
3
4
5
Distance


g(r)
BNT2500K_3_1.74_500ps
0.16
0.12
0.08
0.04
0.00
g(r)
0
1
2
3
4
5
Distance