

```

&FORCE_EVAL
METHOD Quickstep
&DFT
LSD
CHARGE 2
MULTIPLICITY 3
BASIS_SET_FILE_NAME /home/gkr/softwares/cp2k-6.1/data/BASIS_MOLOPT
POTENTIAL_FILE_NAME /home/gkr/softwares/cp2k-6.1/data/GTH_POTENTIALS
WFN_RESTART_FILE_NAME RESTART.wfn
&MGRID
CUTOFF 400
REL_CUTOFF 40
NGRIDS 5
&END MGRID
&QS
METHOD GPW
EPS_DEFAULT 1.0E-12
EXTRAPOLATION ASPC
EXTRAPOLATION_ORDER 3
&END QS
&SCF
MAX_SCF 40
EPS_SCF 1.0E-7
SCF_GUESS RESTART
&OUTER_SCF
EPS_SCF 1.0E-7
MAX_SCF 10
&END OUTER_SCF
&OT
PRECONDITIONER FULL_ALL
MINIMIZER DIIS
N_DIIS 7
&END OT
&END SCF

&XC
&XC_FUNCTIONAL PBE ! PBE functional + ...
&END
&VDW_POTENTIAL ! ... dispersion interactions
POTENTIAL_TYPE PAIR_POTENTIAL
&PAIR_POTENTIAL
TYPE DFTD2 ! computed with the DFTD2 method
REFERENCE_FUNCTIONAL PBE
&END PAIR_POTENTIAL
&END
&END XC
&END DFT

&SUBSYS
&CELL
ABC 12.73 12.73 12.73
PERIODIC XYZ
&END CELL

&COORD
C 0.880000 9.929999 5.500000
C 1.190000 9.000000 6.580000
C 1.690000 7.530000 6.250000
C 1.120000 7.030000 4.870000
C 0.820000 8.000000 3.820000
C 0.740000 9.430000 4.110000
C 1.330000 6.540000 7.420000
C 0.950000 5.610000 4.650000
C 1.000000 4.660000 5.760000
C 1.140000 5.130000 7.140000
C 0.880000 3.230000 5.500000

```

C	0.730000	2.750000	4.130000
C	0.650000	3.710000	3.020000
C	0.720000	5.130000	3.290000
C	0.570000	6.090000	2.190000
C	0.590000	7.530000	2.460000
C	1.070000	9.450000	7.960000
C	1.120000	8.480000	9.060000
C	1.200000	7.040000	8.790000
C	1.130000	6.100000	9.900000
C	1.100000	4.660000	9.630000
C	1.070000	4.190000	8.250000
C	0.900000	2.280000	6.600000
C	0.990000	2.760000	7.990000
C	0.490000	3.240000	1.650000
C	0.400000	4.280000	0.830000
C	0.830000	0.850000	6.320000
C	0.670000	1.320000	3.870000
C	0.740000	0.650000	5.020000
C	0.990000	1.820000	9.100000
C	1.040000	2.480000	10.250000
C	1.070000	3.710000	10.730000
C	1.100000	6.600000	11.280001
C	1.080000	7.920000	11.280001
C	1.050000	8.950000	10.450000
C	0.890000	10.880001	8.230000
C	0.760000	11.540001	7.100000
C	0.700000	11.350000	5.790000
C	0.500000	10.380000	3.020000
C	0.390000	9.720000	1.880000
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C	0.480000	1.910000	1.630000
C	0.560000	1.100000	2.570000
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C	1.090000	4.350000	11.890000
C	1.100000	5.580000	12.120000
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C	0.890000	11.090000	9.540000
C	0.390000	5.600000	0.830000
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C	4.280000	6.810000	6.040000
C	4.400000	5.370000	6.060000
C	5.470000	7.500000	5.920000
C	5.680000	4.780000	5.920000
H	3.550000	4.740000	6.190000
C	6.600000	6.850000	5.830000
H	5.480000	8.550000	5.920000
H	5.800000	3.700000	5.900000
N	6.770000	5.580000	5.820000
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C	8.090000	8.770000	5.690000
N	8.750000	6.520000	5.650000
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O	10.050000	4.130000	5.850000
O	9.180000	4.460000	3.660000
O	9.180000	4.630000	7.440000
C	9.400000	9.190001	5.620000
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C	10.039999	6.850000	5.570000
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C	10.369999	8.230000	5.570000
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H	10.727179	7.698723	9.628339
H	9.844040	12.057049	6.669122
O	8.355300	5.545262	10.908658
H	8.976822	6.278328	10.721400
H	7.695647	5.712935	10.201671
O	11.192607	4.774025	11.445318
H	10.545305	4.746277	12.232038
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O	3.966201	4.931618	3.399235
H	3.643015	4.313115	4.046968
H	4.882634	4.814923	3.248324
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H	7.534626	9.782350	9.806070
H	7.622112	10.496266	11.287123
O	12.450509	7.616537	11.145765
H	12.606269	8.113300	12.349998
H	12.411700	6.644406	10.931167
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H	10.826283	12.325910	5.583535
H	11.122058	11.121305	7.830110
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H	8.290289	3.805989	10.694123
H	8.527999	2.825292	11.903119
O	6.768320	7.895758	11.054452
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H	5.766282	12.348249	2.356647
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H	3.293218	11.546611	4.804966
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H	7.245504	12.322224	4.436040
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O	3.841299	11.295623	8.386219
H	4.321449	11.061031	7.486182

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&END COORD

&KIND H
BASIS_SET DZVP-MOLOPT-SR-GTH-q1
POTENTIAL GTH-PBE-q1
&END KIND
&KIND C
BASIS_SET DZVP-MOLOPT-SR-GTH-q4
POTENTIAL GTH-PBE-q4
&END KIND
&KIND N
BASIS_SET DZVP-MOLOPT-SR-GTH-q5
POTENTIAL GTH-PBE-q5
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&KIND O
BASIS_SET DZVP-MOLOPT-SR-GTH-q6
POTENTIAL GTH-PBE-q6
&END KIND
&KIND Co
BASIS_SET DZVP-MOLOPT-SR-GTH-q17
POTENTIAL GTH-PBE-q17
&END KIND
&END SUBSYS
&END FORCE_EVAL

&GLOBAL
PROJECT co-graphene-nvt
RUN_TYPE MD
PRINT_LEVEL LOW
&END GLOBAL

&MOTION
&MD
ENSEMBLE NVT
STEPS 10000
TIMESTEP 0.5
TEMPERATURE 300
TEMP_TOL 10
&THERMOSTAT
&NOSE
LENGTH 3
YOSHIDA 3
TIMECON 30.0
MTS 2
&END NOSE
&END
&END MD

&PRINT
&TRAJECTORY SILENT

COMMON_ITERATION_LEVELS	3
&END TRAJECTORY	
&CELL SILENT	
COMMON_ITERATION_LEVELS	3
&END CELL	
&VELOCITIES SILENT	
COMMON_ITERATION_LEVELS	3
&END VELOCITIES	
&RESTART SILENT	
COMMON_ITERATION_LEVELS	3
&END RESTART	
&END PRINT	
&END MOTION	