&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

C 0.390000 8.500000 1.380000

C 0.520000 12.030000 4.670000

C 0.440000 11.619999 3.490000

C 0.270000 7.850000 0.230000

C 0.260000 6.620000 0.000000

C 0.480000 1.910000 1.630000

C 0.560000 1.100000 2.570000

C 0.870000 0.170000 7.460000

C 0.940000 0.570000 8.640000

C 1.090000 4.350000 11.890000

C 1.100000 5.580000 12.120000

C 0.960000 10.270000 10.480000

C 0.890000 11.090000 9.540000

C 0.390000 5.600000 0.830000

N 3.180000 7.650000 6.080000

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

C 7.870000 7.450000 5.720000

C 8.090000 8.770000 5.690000

N 8.750000 6.520000 5.650000

O 8.230000 2.960000 5.670000

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

H 7.280000 9.450000 5.730000

C 10.039999 6.850000 5.570000

H 8.809999 2.200000 5.770000

H 10.080000 4.490000 3.350000

H 8.750000 3.650000 3.380000

H 10.130000 4.640000 7.620000

H 8.809999 3.810000 7.780000

C 10.369999 8.230000 5.570000

H 9.639999 10.240001 5.620000

H 10.809999 6.090000 5.510000

H 11.400000 8.530000 5.530000

Co 8.430000 4.710000 5.530000

O 10.747491 7.590243 8.598937

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

H 11.270716 3.906816 10.943052

O 3.966201 4.931618 3.399235

H 3.643015 4.313115 4.046968

H 4.882634 4.814923 3.248324

O 7.986815 10.461365 10.380076

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

O 6.897713 3.008714 8.713646

H 6.511094 3.381194 9.557111

H 7.322736 2.196355 9.002359

O 5.777533 2.701413 1.205623

H 5.029792 3.318140 1.117399

H 5.794541 2.248563 0.343773

O 4.097491 3.236042 8.248528

H 3.985621 4.041606 8.810557

H 5.093555 3.163145 8.206713

O 10.843990 12.260831 6.575796

H 10.826283 12.325910 5.583535

H 11.122058 11.121305 7.830110

O 8.586997 2.854648 10.921709

H 8.290289 3.805989 10.694123

H 8.527999 2.825292 11.903119

O 6.768320 7.895758 11.054452

H 7.478734 7.929360 11.731563

H 7.287490 7.824143 10.231608

O 3.874013 8.684276 8.743598

H 3.634863 8.290987 7.873202

H 3.557733 9.618033 8.694829

O 6.011199 -0.343796 9.399488

H 5.201989 -0.959132 9.292953

H 6.668013 -1.036566 9.690725

O 6.897567 2.493233 3.682509

H 7.234938 2.467649 4.559132

H 6.137557 1.882025 3.438478

O 10.253689 12.982252 4.079344

H 9.435786 12.515319 4.338540

H 10.543897 12.493642 3.284178

O 12.301828 11.974570 12.562934

H 11.980198 12.125349 11.597016

H 12.464193 11.017178 12.589131

O 10.597003 2.405199 2.645597

H 10.334195 1.610062 3.179177

H 11.332718 2.750455 3.107687

O 10.773828 1.603800 -0.086868

H 10.806158 1.956165 0.811919

H 11.726752 1.621472 -0.341964

O 10.654727 6.924871 2.718303

H 10.620008 7.907376 2.706496

H 9.709547 6.850519 3.073702

O 10.732882 10.077434 11.246646

H 9.762946 9.915641 11.050227

H 11.176422 9.246428 11.423914

O 2.961173 2.406630 12.598989

H 3.179674 3.346006 12.991539

H 3.172288 2.058818 13.519256

O 5.776417 12.536417 3.375795

H 5.766282 12.348249 2.356647

H 4.890325 12.539184 3.846558

O 3.879960 10.264947 2.087164

H 3.591460 9.491004 1.531560

H 3.529678 8.961095 5.081512

O 3.873634 0.884195 7.094145

H 4.835124 0.912930 7.146903

H 3.576238 1.717304 7.537430

O 10.755840 10.360808 8.342281

H 10.937420 10.529557 9.260922

H 11.157245 8.431048 8.285234

O 2.824619 11.574911 11.494320

H 3.501506 10.889529 11.570793

H 3.343955 12.344353 11.081221

O 2.407824 12.219968 1.190987

H 3.107658 10.959175 1.974846

H 2.648231 11.958112 0.218929

O 11.422143 12.661217 10.021826

H 10.499134 12.330298 10.131231

H 11.225121 13.670368 9.949944

O 6.681015 9.522381 3.124437

H 5.731445 9.743104 3.103454

H 7.058577 10.294245 3.619314

O 5.787589 7.928681 0.720673

H 6.367018 8.645560 0.973476

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O 4.159175 6.454400 11.682593

H 4.950068 6.985016 11.855124

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H 8.209251 7.586437 1.246606

O 3.731437 1.315200 10.187983

H 3.995164 1.789544 9.423810

H 3.621844 1.979105 10.957786

O 3.910918 2.668686 4.586197

H 3.647894 2.239578 5.400266

H 3.579634 2.154469 3.850236

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H 4.703105 10.419343 5.516718

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H 6.589850 1.686881 7.100865

O 4.480165 7.451674 3.091281

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H 5.179364 7.378059 2.332794

O 8.242700 2.989244 0.800732

H 7.381610 3.434374 1.080958

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H 8.596127 0.674694 10.013165

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O 7.883119 7.223924 2.856329

H 7.368552 6.392552 3.056608

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O 4.612465 9.470360 11.387348

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H 5.614794 9.105819 11.314048

O 6.319296 9.305797 8.286256

H 6.203575 10.025149 7.509885

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O 3.532145 12.559317 4.611544

H 3.355182 12.883183 5.534250

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O 10.910221 2.506111 9.871119

H 10.001445 2.736092 10.285110

H 10.724571 2.572903 8.928989

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H 8.437132 1.405442 1.222127

H 7.839385 0.691211 2.480533

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H 10.443686 2.701953 6.516008

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H 9.764090 12.499016 1.548346

H 11.204437 12.077744 0.952184

O 3.841299 11.295623 8.386219

H 4.321449 11.061031 7.486182

H 3.481776 12.217567 8.176330

O 6.431921 4.962752 2.998924

H 6.469556 5.068657 1.996485

H 6.773592 3.883811 2.971516

O 6.884172 5.372813 0.484062

H 6.573124 5.138368 -0.408561

H 6.653374 6.305342 0.694114

O 5.528439 11.805328 0.691237

H 4.721204 11.353884 1.039205

H 5.348190 12.477672 0.001024

O 6.533318 5.636213 8.695601

H 7.221125 6.362147 8.491354

H 6.785088 4.822701 8.264505

O 7.926146 10.826122 0.202004

H 8.627344 10.492409 0.845892

H 7.132014 11.275638 0.628410

&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

&END KIND

&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