&FORCE\_EVAL

METHOD Quickstep

&DFT

LSD

CHARGE 2

MULTIPLICITY 3

BASIS\_SET\_FILE\_NAME /home/softwares/cp2k-6.1/data/BASIS\_MOLOPT

POTENTIAL\_FILE\_NAME /home/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 12.404098 9.332770 9.447946

H 11.923949 8.499675 9.068308

H 12.162019 9.897792 9.097250

O 8.286545 5.348079 10.851565

H 9.069373 5.949940 10.693591

H 7.726088 5.415790 10.071713

O 11.281870 5.050102 10.869153

H 10.737642 4.765806 11.633730

H 11.177316 4.574296 10.044624

O 3.588240 5.606637 3.146801

H 3.263690 5.362759 4.040280

H 4.579387 5.412274 3.117908

O 5.857522 10.711571 10.624726

H 6.402214 10.239841 9.914412

H 6.409789 10.675488 11.467713

O 12.366385 12.058693 12.824754

H 13.399948 11.925178 12.969203

H 11.961684 11.114391 12.716013

O 6.707994 3.479222 8.839972

H 6.611348 3.347001 9.798984

H 7.432682 2.887933 8.484090

O 5.471995 2.373734 1.772371

H 4.753633 3.026297 1.507735

H 5.392340 1.633820 1.098818

O 3.955551 3.816030 8.363642

H 3.819342 4.751440 8.633911

H 4.933250 3.770520 8.372482

O 10.544162 11.751232 7.400161

H 10.724796 12.192279 6.516649

H 10.781874 10.732900 7.532798

O 9.669894 2.602030 10.525193

H 9.044835 3.305825 10.868420

H 10.166478 2.294454 11.349806

O 7.034010 8.274551 10.885018

H 6.980515 7.518046 10.249358

H 7.440249 7.949741 11.706105

O 4.284448 9.162192 8.663743

H 3.657076 8.697364 8.058378

H 4.145706 10.070763 8.498639

O 5.972058 0.614543 9.218296

H 5.314219 1.223690 9.647124

H 6.198081 -0.058803 9.860693

O 7.355778 2.533702 3.268481

H 7.611379 2.362614 4.261191

H 6.473466 2.227802 2.962226

O 10.331949 12.387435 4.762896

H 9.362175 12.118032 4.981767

H 10.530723 12.037282 3.828362

O 10.845941 10.062298 12.029486

H 10.890564 9.158543 11.706609

H 10.132658 10.404480 11.395255

O 10.289761 1.998159 2.897460

H 9.851845 1.556696 3.663063

H 11.180053 1.633564 2.941514

O 10.764009 2.039192 0.068647

H 10.109786 1.762525 0.759856

H 11.495730 1.355284 -0.003068

O 10.418432 6.562651 2.649082

H 10.891055 7.340462 2.259623

H 9.472508 6.845689 2.818567

O 8.904014 10.187630 10.391479

H 8.540599 10.805346 9.657059

H 8.116128 9.522020 10.577090

O 3.191913 1.662600 12.914807

H 3.191911 2.428343 13.515638

H 4.304636 1.502898 12.819210

O 5.988401 12.901939 4.207874

H 5.852409 12.472088 3.338287

H 5.114140 13.014837 4.627586

O 3.416808 9.678453 1.758075

H 3.519938 8.804147 1.318326

H 3.234285 9.752371 3.501006

O 3.650465 1.823495 6.530085

H 4.633223 1.649881 6.528234

H 3.579216 2.663052 7.078559

O 10.991426 9.435291 8.541409

H 10.302110 9.597089 9.235606

H 11.138089 8.451505 8.350898

O 3.662198 12.200349 11.056360

H 4.405170 11.616640 10.667486

H 3.422035 12.801785 10.347300

O 2.323884 11.572591 0.396734

H 2.826215 10.342841 1.171566

H 2.783895 11.797350 -0.430060

O 11.086710 12.944433 9.897257

H 11.102164 12.625845 8.957537

H 11.130258 12.162741 10.490171

O 8.115506 10.487190 3.276587

H 7.231500 10.028698 3.326102

H 8.302737 10.951592 4.129316

O 5.860290 8.471178 0.589910

H 6.477704 9.222869 0.625578

H 5.276190 8.578064 -0.192504

O 4.138031 5.365257 11.739085

H 5.150601 5.351523 11.884815

H 4.011102 5.652783 10.809882

O 7.985861 0.986660 11.054819

H 8.376000 0.131301 10.926792

H 8.539503 1.688649 10.642510

O 3.018234 7.096655 0.743694

H 3.563628 6.702924 0.014992

H 3.120881 6.403535 1.475402

O 8.992762 7.920679 0.389080

H 9.579092 8.522217 0.958306

H 8.445730 7.474398 1.111896

O 3.975399 2.142374 10.325369

H 3.857405 3.055978 9.848350

H 3.647168 2.176110 11.312949

O 3.692770 2.918682 3.989937

H 3.707637 2.459240 4.846477

H 4.427780 2.551426 3.467799

O 3.969370 6.547176 9.249332

H 3.875604 7.491505 9.610918

H 4.923296 6.492752 9.026237

O 11.151983 6.841617 8.101723

H 11.465461 6.076881 8.670675

H 10.183317 6.959433 8.325113

O 3.267934 0.251437 2.479259

H 3.469419 1.174743 2.391759

H 4.059345 -0.316670 2.165128

O 8.111323 11.726496 8.306863

H 9.082364 11.683496 8.030562

H 8.074693 12.707514 8.293646

O 8.693889 7.526555 8.778485

H 9.219491 7.844552 9.580883

H 8.163457 8.292822 8.490111

O 5.424429 10.506447 6.162764

H 5.787641 11.295341 5.690533

H 4.694456 10.930717 6.680227

O 6.166491 1.418694 6.774884

H 6.404363 1.143599 7.704788

H 6.835497 1.986150 6.301281

O 5.952466 8.826712 3.330177

H 5.281934 9.335298 3.912863

H 5.538922 8.878300 2.456667

O 8.236210 3.035979 0.480203

H 7.884389 2.808025 1.338816

H 8.354776 4.050630 0.572938

O 8.706095 1.661384 8.202447

H 9.130429 1.805014 9.100825

H 9.510016 1.667252 7.620523

O 7.848607 7.120775 2.844564

H 7.310173 6.286022 2.752607

H 7.151304 7.771294 3.156344

O 4.057541 8.732594 11.387761

H 3.319571 9.328631 11.641226

H 4.655971 9.354863 10.833034

O 6.835819 9.251141 8.334820

H 6.956151 10.068217 7.813367

H 5.841970 9.051936 8.350775

O 5.600779 0.470934 12.541497

H 6.400403 0.223457 12.017491

H 4.724747 0.343262 12.028705

O 3.626088 9.684929 4.373911

H 2.153409 10.382459 0.877483

H 3.504357 10.556325 4.809592

O 3.519336 3.923479 1.202995

H 3.342250 4.437770 2.018883

H 3.705929 4.503144 0.377193

O 10.071483 5.079258 0.620781

H 10.278063 4.242037 0.971132

H 10.091964 5.744727 1.413649

O 10.081756 9.166545 2.151982

H 9.374416 9.579218 2.642653

H 10.603825 9.888906 1.776797

O 6.360941 3.438975 11.367216

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H 5.595289 2.811101 11.344168

O 3.543402 12.340779 5.118610

H 3.101452 12.935148 5.752086

H 3.184027 12.738461 4.243097

O 11.119641 3.656857 8.568848

H 10.527477 3.102559 9.198110

H 11.447110 3.006655 7.888286

O 8.231526 0.174907 1.453484

H 8.187306 0.421990 0.510026

H 8.085561 0.926131 2.034170

O 10.689381 1.835545 6.498428

H 10.610376 1.171898 5.792626

H 10.469232 2.793992 6.108580

O 10.460902 7.584771 10.858984

H 9.854880 7.529925 11.627604

H 10.787142 6.644705 10.854403

O 7.964292 11.885375 5.661053

H 7.289601 12.445894 5.187976

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O 10.733572 11.851904 2.130014

H 9.914248 12.228116 1.880153

H 11.387501 12.186364 1.496648

O 3.956469 11.810072 7.914109

H 4.787072 12.419822 8.110357

H 3.113430 12.304714 7.928323

O 6.155239 5.069290 2.905355

H 6.199959 5.114939 1.903559

H 6.540957 4.231854 3.142246

O 6.492074 5.858118 0.223028

H 7.192448 5.945185 -0.418825

H 6.212898 6.797228 0.430303

O 5.354506 11.481859 1.859102

H 4.745312 10.713911 1.583958

H 5.671007 12.070744 1.115976

O 6.577593 6.163820 8.799687

H 7.483995 6.539760 8.545852

H 6.560746 5.291751 8.417702

O 7.550302 10.463799 0.236409

H 8.215593 9.702062 0.192101

H 7.842514 11.005569 1.022850

&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-oh-oxo-nve

RUN\_TYPE MD

PRINT\_LEVEL LOW

&END GLOBAL

&MOTION

&CONSTRAINT

&FIXED\_ATOMS

COMPONENTS\_TO\_FIX XYZ

LIST 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84

&END FIXED\_ATOMS

&END CONSTRAINT

&MD

ENSEMBLE NVE

STEPS 10000

TIMESTEP 0.5

TEMPERATURE 300

TEMP\_TOL 05

&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