M-SPARC and KSSOLV Simulations

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In this live script we showcase 2 DFT community toolboxes, M-SPARC and KSSOLV. These are Kohn-Sham DFT solvers in real-space and momemtum-space using plane wave basis, respectively. Both toolboxes are 3-Dimensional pseudopotential implementation of Kohn-Sham theory and can work with norm-conserving pseudopotentials in psp8 format. Here we use the default pseudopotential files porvided within the toolboxes. We need 2 toolboxes to be downloaded and installed, with their paths added properly. To download the toolboxes, use the following links: https://github.com/SPARC-X/M-SPARC for M-SPARC and https://bitbucket.org/berkeleylab/kssolv2.0/src/release/ for KSSOLV. After downloading the toolboxes, put their paths below. Don't remove the M-SPARC/ and KSSOLV/ folder in the directory. Afterwards, you can start the simulations.

```
MSPARC_root = 'C:\...\DFTMaterial\M-SPARC';
KSSOLV_root = 'C:\...\DFTMaterial\kssolv2.0';

if ~exist('M-SPARC', 'dir') || ~exist('KSSOLV', 'dir')
   error('Do not remove M-SPARC/ and KSSOLV/ folder!');
end
```

Monoatomic Molecules (Atoms)

We start with simulating a monoatomic molecule, an atom. First we select atom symbol and specify linear size (length) of the finite simulation cube in units of Bohr radius. The atom will be placed at the center of the cube. The cube should be sufficiently large to achieve desired accuracy.

```
atom = 'He'; % atom symbol
L1 = 20;   % linear size of unit cell in Bohr radius
```

For M-SPARC, here we select mesh size (step size) in real space in units of Bohr radius. In practice, we need to do a mesh convergence test to get an accurate result.

```
h1 = 0.2; % in Bohr
% path and check
addpath(MSPARC_root);
addpath(fullfile(MSPARC_root,"src"));
addpath("M-SPARC\");
% Real space toolbox M-SPARC
msparc_monoatomMol(atom,L1,h1,MSPARC_root);
S1 = msparc("M-SPARC/monoatom");
```

```
 Reading .inpt file ...


<INPT>
# $ cat M-SPARC/monoatom.inpt
LATVEC_SCALE: 20.000000 20.000000 20.000000
MESH_SPACING: 0.200000
BC: D D D
EXCHANGE_CORRELATION: GGA_PBE
<\INPT>

 Reading .ion file ...
 Number of atom types : 1
 Total number of atoms: 1
 Default atomic mass for He is 4.002602
 pseudo_dir # 1 = 02_He_2_1.1_1.2_pbe_v1.0.psp8

 COORD:
    10    10    10

atom type 1, l = 0, r_core read 1.25127, change to rmax where |UdV| < 1E-8, 1.27000.
atom type 1, l = 1, r_core read 1.13028, change to rmax where |UdV| < 1E-8, 1.15000.
 reduced kpoint grid before symmetry:
     0     0     0

 reduced kpoint grid after symmetry:
     0     0     0

 nspin = 1, nspinor = 1, nspden = 1
## Chebyshev polynomial degree not provided, finding npl ...
## Based on the mesh size, npl is set to: 35
## Number of states not provided, finding Nev ...
## Based on the number of electrons, Nev is set to: 6
## Based on the desired accuracy, SCF_tol is set to: 2.159e-04
## Poisson tolerance not provided, choosing poisson_tol ...
## poisson_tol is set to: 2.159e-06
## Pseudocharge tolerance not provided, choosing pseudocharge_tol ...
## pseudocharge_tol is set to: 2.159e-07
 Creating differentiation matrices ...
 Done. (4.653 sec)

 Estimated memory usage:
 Total:    3.81 GB
 orbitals            :  141.49 MB
 sparse matrices     :    2.53 GB
 global-size vectors :  143.07 MB
 spherical harmonics :  924.58 MB
 mixing histories    :  110.05 MB

 Finding rb for He ...
 rb = {1.600 1.600 1.600}, int_b = -1.999944523453230, err_rb = 5.548e-05
 rb = {1.800 1.800 1.800}, int_b = -2.000020618950575, err_rb = 2.062e-05
 rb = {2.000 2.000 2.000}, int_b = -2.000005610661231, err_rb = 5.611e-06
 rb = {2.200 2.200 2.200}, int_b = -2.000003610704292, err_rb = 3.611e-06
 rb = {2.400 2.400 2.400}, int_b = -2.000003255390591, err_rb = 3.255e-06
 rb = {2.600 2.600 2.600}, int_b = -2.000004232434032, err_rb = 4.232e-06
 rb = {2.800 2.800 2.800}, int_b = -2.000005776064260, err_rb = 5.776e-06
 rb = {3.000 3.000 3.000}, int_b = -2.000007332397191, err_rb = 7.332e-06
 rb = {3.200 3.200 3.200}, int_b = -2.000008603018708, err_rb = 8.603e-06
 rb = {3.400 3.400 3.400}, int_b = -2.000009625856349, err_rb = 9.626e-06
 rb = {3.600 3.600 3.600}, int_b = -2.000010484569035, err_rb = 1.048e-05
 rb = {3.800 3.800 3.800}, int_b = -2.000011115609907, err_rb = 1.112e-05
 rb = {4.000 4.000 4.000}, int_b = -2.000012017599960, err_rb = 1.202e-05
 rb = {4.200 4.200 4.200}, int_b = -2.000013042426987, err_rb = 1.304e-05
```

```
rb = {4.400 4.400 4.400}, int_b = -2.000012980161126, err_rb = 1.298e-05
rb = {4.600 4.600 4.600}, int_b = -2.000011559458235, err_rb = 1.156e-05
rb = {4.800 4.800 4.800}, int_b = -2.000010233206323, err_rb = 1.023e-05
rb = {5.000 5.000 5.000}, int_b = -2.000009940388191, err_rb = 9.940e-06
rb = {5.200 5.200 5.200}, int_b = -2.000009635216004, err_rb = 9.635e-06
rb = {5.400 5.400 5.400}, int_b = -2.000007566303623, err_rb = 7.566e-06
rb = {5.600 5.600 5.600}, int_b = -2.000007464478120, err_rb = 7.464e-06
rb = {5.800 5.800 5.800}, int_b = -2.000007346995559, err_rb = 7.347e-06
rb = {6.000 6.000 6.000}, int_b = -1.999999034906817, err_rb = 9.651e-07
rb = {6.200 6.200 6.200}, int_b = -2.000000200536177, err_rb = 2.005e-07
rb = {6.200 6.200 6.200}

###################################################################
Relaxation step number: 1

WARNING: REFERENCE _CUFOFF (0.500000 Bohr) > 1/2 nn (nearest neighbor) distance (0.000000 Bohr) in SCF#1

Starting pseudocharge generation and self energy calculation...
Integration b = 2.000000200536

Integration b_ref = 2.000000000001

**************************************
*          Eself_ref = 7.140299       *
**************************************
Done. (0.183425 s)
Time for b calculation: 0.218 seconds.

Starting calculating nonlocal projectors ...
Done. (0.026236 s)

~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
Starting SCF iteration...
AAR converged to a relative residual of 9.29844e-07 in 157 iterations.
Poisson problem took 25.182430s
==========================================
Relaxation iteration:  1
SCF iteration number:  1, Chebyshev cycle: 1
==========================================
Fermi energy = 3.925851
==========================================
Relaxation iteration:  1
SCF iteration number:  1, Chebyshev cycle: 2
==========================================
Fermi energy = 0.537920
==========================================
Relaxation iteration:  1
SCF iteration number:  1, Chebyshev cycle: 3
==========================================
Fermi energy = 0.148234
==========================================
Relaxation iteration:  1
SCF iteration number:  1, Chebyshev cycle: 4
==========================================
Fermi energy = 0.047467
------------------
Eband = -1.15808210
Exc = -1.01622254
Exc_dc = -1.30244419
Eelec_dc = 0.88220389
Eent = -0.00000001
E_corr = 0.00000003
Eself = 2.86318074
Etot = -2.85283727
```

```
 ------------------
 Etot = -2.85283727
 Eatom = -2.85283727
 Error in SCF iteration: 1.4398e-03
 AAR converged to a relative residual of 2.769e-05 in 31 iterations.

Density got negative

 AAR converged to a relative residual of 1.92542e-06 in 49 iterations.
 Poisson problem took 8.335377s
 This SCF iteration took 75.727 s.

 ========================
 Relaxation iteration:  1
 SCF iteration number:  2
 ========================
 Fermi energy = 0.018806
 ------------------
 Eband = -1.15869748
 Exc = -1.01608602
 Exc_dc = -1.30226743
 Eelec_dc = 0.88251476
 Eent = -0.00000001
 E_corr = 0.00000003
 Eself = 2.86318074
 Etot = -2.85318202
 ------------------
 Etot = -2.85318202
 Eatom = -2.85318202
 Error in SCF iteration: 3.5705e-04
 AAR converged to a relative residual of 2.82026e-05 in 25 iterations.

Density got negative

 AAR converged to a relative residual of 2.01271e-06 in 19 iterations.
 Poisson problem took 3.713977s
 This SCF iteration took 19.715 s.

 ========================
 Relaxation iteration:  1
 SCF iteration number:  3
 ========================
 Fermi energy = 0.007758
 ------------------
 Eband = -1.15865265
 Exc = -1.01611435
 Exc_dc = -1.30230384
 Eelec_dc = 0.88245872
 Eent = -0.00000001
 E_corr = 0.00000003
 Eself = 2.86318074
 Etot = -2.85318516
 ------------------
 Etot = -2.85318516
 Eatom = -2.85318516
 Error in SCF iteration: 3.3544e-04
 AAR converged to a relative residual of 1.8507e-05 in 25 iterations.

Density got negative

 AAR converged to a relative residual of 1.79339e-06 in 25 iterations.
 Poisson problem took 4.631963s
 This SCF iteration took 20.702 s.
```

```
 ========================
 Relaxation iteration:  1
 SCF iteration number:  4
 ========================
 Fermi energy = 0.002513
 ------------------
 Eband = -1.15860327
 Exc = -1.01614210
 Exc_dc = -1.30233955
 Eelec_dc = 0.88240127
 Eent = -0.00000001
 E_corr = 0.00000003
 Eself = 2.86318074
 Etot = -2.85318525
 ------------------
 Etot = -2.85318525
 Eatom = -2.85318525
 Error in SCF iteration: 2.2465e-04
 AAR converged to a relative residual of 3.66413e-05 in 20 iterations.

Density got negative

 AAR converged to a relative residual of 1.51837e-06 in 31 iterations.
 Poisson problem took 5.577804s
 This SCF iteration took 20.802 s.

 ========================
 Relaxation iteration:  1
 SCF iteration number:  5
 ========================
 Fermi energy = -0.000143
 ------------------
 Eband = -1.15855212
 Exc = -1.01616982
 Exc_dc = -1.30237531
 Eelec_dc = 0.88234205
 Eent = -0.00000001
 E_corr = 0.00000003
 Eself = 2.86318074
 Etot = -2.85318530
 ------------------
 Etot = -2.85318530
 Eatom = -2.85318530
 Error in SCF iteration: 1.0599e-04
 AAR converged to a relative residual of 3.02586e-05 in 25 iterations.

Density got negative

 AAR converged to a relative residual of 2.15097e-06 in 31 iterations.
 Poisson problem took 5.499955s
 This SCF iteration took 21.517 s.


 Finished SCF iteration in 5 steps!
 ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~

 ********************************************************
 *          Energy per unit cell = -2.853185300 Ha.       *
 *          Energy per atom = -2.853185300 Ha.            *
 ********************************************************

 Starting atomic force calculation ...
 local force calculation: 0.310 s
 ********************************************************
```

```
*                      Atomic Force                      *
*********************************************************
Drift free forces (Ha/Bohr):
    0     0     0

Max magnitude of forces (Ha/Bohr):     0


Time for calculating forces: 2.076213 s.
~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
Final atomic positions (Cartesian) are as follows:
10.000000      10.000000      10.000000

Run-time of the program: 196.272585 seconds
```

```
rmpath(MSPARC_root);
rmpath(fullfile(MSPARC_root,"src"));
rmpath("M-SPARC\");
```

Here we choose Kinetic energy cutoff in momentum space E_{cut} in units of Hartree for KSSOLV. Usually, we need to perform convergence test in E_{cut} as well.

```
Ecut1 = 20; % in Ha

% path and check
addpath(KSSOLV_root);
addpath("KSSOLV\");
KSSOLV_startup;
[K_mol1,K_Ham1,K_wf1,K_info1] = kssolv_monoatomMol(atom,L1,Ecut1);
```

```
The pseudopotential for He is loaded from C:\Users\tvekua\OneDrive - MathWorks\Desktop\DFTMaterial\KSSOLV\/ppdata/de
The pseudopotential for He is loaded from C:\Users\tvekua\OneDrive - MathWorks\Desktop\DFTMaterial\KSSOLV\/ppdata/de
Regular SCF for Pure DFT
Beging SCF calculation for He...
SCF iter   1:
eigtol =   1.000e-02
Rel Vtot Err    =            5.856e-02
Total Energy    = -2.7904730741642e+00
SCF iter   2:
eigtol =   1.000e-02
Rel Vtot Err    =            1.173e-02
Total Energy    = -2.7904731226360e+00
SCF iter   3:
eigtol =   5.867e-03
Rel Vtot Err    =            1.389e-04
Total Energy    = -2.7904731236473e+00
SCF iter   4:
eigtol =   6.943e-05
Rel Vtot Err    =            4.708e-05
Total Energy    = -2.7904731236658e+00
SCF iter   5:
eigtol =   2.354e-05
Rel Vtot Err    =            7.349e-07
Total Energy    = -2.7904731236661e+00
SCF iter   6:
eigtol =   3.675e-07
Rel Vtot Err    =            2.327e-08
Total Energy    = -2.7904731236661e+00
SCF iter   7:
```

```
eigtol =   1.164e-08
Rel Vtot Err    =            1.853e-10
Total Energy    = -2.7904731236661e+00
Convergence is reached!
resnrm =   3.864e-11
---------------------
Elapsed time is 12.555770 seconds.
Etot            = -2.7904731236661e+00
Eone-electron   = -3.1557247392633e+00
Ehartree        =  1.6262467264379e+00
Exc             = -9.7726533576073e-01
Eewald          = -2.8372977508004e-01
Ealphat         =  0.0000000000000e+00
-------------------------------------
Total time used =            1.517e+01
||HX-XD||_F     =            3.864e-11
```

```
rmpath(KSSOLV_root);
rmpath("KSSOLV\");
fprintf("Total energy of single atom %s molecule from M-SPARC is %.6f Ha\n", atom,
S1.Etotal);
```

```
Total energy of single atom He molecule from M-SPARC is -2.853185 Ha
```

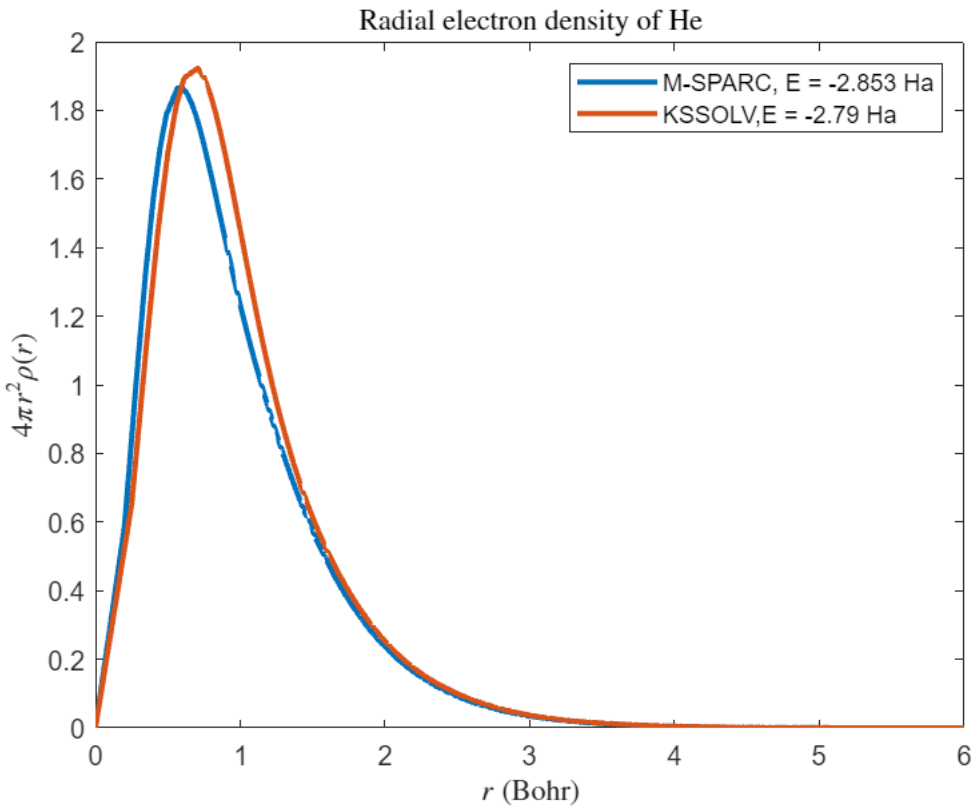
```
fprintf("Total energy of single atom %s molecule from KSSOLV is %.6f Ha\n", atom,
K_info1.Etot);
```

```
Total energy of single atom He molecule from KSSOLV is -2.790473 Ha
```

Next, we visualize the radial electron density obtained from 2 toolboxes below.

```
% M-SPARC
rhom = S1.rho(:,1);
x = linspace(-L1/2,L1/2,S1.Nx);
y = linspace(-L1/2,L1/2,S1.Ny);
z = linspace(-L1/2,L1/2,S1.Nz);
[X,Y,Z] = ndgrid(x,y,z);
[~,~,Rm] = cart2sph(X,Y,Z);
Rm = Rm(:);
rrhom = 4*pi*Rm.^2.*rhom;
[Rm,~,indx] = unique(Rm);
rrhom = accumarray(indx, rrhom, [], @mean);

% KSSOLV
rhok = reshape(fftshift(K_Ham1.rho),[],1);
x = linspace(-L1/2,L1/2,K_Ham1.n1);
y = linspace(-L1/2,L1/2,K_Ham1.n2);
z = linspace(-L1/2,L1/2,K_Ham1.n3);
[X,Y,Z] = ndgrid(x,y,z);
[~,~,Rk] = cart2sph(X,Y,Z);
Rk = Rk(:);
rrhok = 4*pi*Rk.^2.*rhok;
[Rk,~,indx] = unique(Rk);
rrhok = accumarray(indx, rrhok, [], @mean);
```

```
figure
plot(Rm,rrhom,Rk,rrhok,'LineWidth',2)
legend("M-SPARC, E = " + num2str(S1.Etotal,4) + " Ha","KSSOLV,E = " +
num2str(K_info1.Etot,4) + " Ha")
xlabel("$r$ (Bohr)",'Interpreter','latex')
ylabel("$4\pi r^2 \rho(r)$",'Interpreter','latex')
title(['Radial electron density of ', atom],'Interpreter','latex')
xlim([0 6])
```



Diatomic Molecules

Next, we present the calculation on diatomic molecules using 2 toolboxes. We can select 2 atoms from the dropbox below. Again we need to define the linear size of the simulation cube and the bond length d in Bohr.

```
atom1 = 'Na'; % atom1 symbol
atom2 = 'Cl'; % atom2 symbol
L2 = 12; % in Bohr
d = 2;  % in Bohr
```

We select the mesh spacing in real-space below.

```
h2 = 0.3; % in Bohr

addpath(MSPARC_root);
addpath(fullfile(MSPARC_root,"src"));
addpath("M-SPARC\");
```

```
% Real space toolbox M-SPARC
msparc_diatomMol(atom1,atom2,L2,d,h2,MSPARC_root);
S2 = msparc("M-SPARC/diaatom");
```

```
 Reading .inpt file ...


<INPT>
# $ cat M-SPARC/diaatom.inpt
LATVEC_SCALE: 12.000000 12.000000 12.000000
MESH_SPACING: 0.300000
BC: D D D
EXCHANGE_CORRELATION: GGA_PBE
<\INPT>

 Reading .ion file ...
 Number of atom types : 2
 Total number of atoms: 2
 Default atomic mass for Na is 22.989769
 Default atomic mass for Cl is 35.451500
 pseudo_dir # 1 = 11_Na_9_1.8_2.2_pbe_v1.0.psp8
 pseudo_dir # 2 = 17_Cl_7_1.9_1.9_pbe_n_v1.0.psp8

 COORD:
     5     6     6
     7     6     6

atom type 1, l = 0, r_core read 1.77096, change to rmax where |UdV| < 1E-8, 1.79000.
atom type 1, l = 1, r_core read 2.20971, change to rmax where |UdV| < 1E-8, 2.22000.
atom type 2, l = 0, r_core read 1.90538, change to rmax where |UdV| < 1E-8, 1.92000.
atom type 2, l = 1, r_core read 1.87149, change to rmax where |UdV| < 1E-8, 1.89000.
atom type 2, l = 2, r_core read 1.90538, change to rmax where |UdV| < 1E-8, 1.92000.
 reduced kpoint grid before symmetry:
     0     0     0

 reduced kpoint grid after symmetry:
     0     0     0

 nspin = 1, nspinor = 1, nspden = 1
## Chebyshev polynomial degree not provided, finding npl ...
## Based on the mesh size, npl is set to: 25
## Number of states not provided, finding Nev ...
## Based on the number of electrons, Nev is set to: 15
## Based on the desired accuracy, SCF_tol is set to: 2.159e-04
## Poisson tolerance not provided, choosing poisson_tol ...
## poisson_tol is set to: 2.159e-06
## Pseudocharge tolerance not provided, choosing pseudocharge_tol ...
## pseudocharge_tol is set to: 2.159e-07
 Creating differentiation matrices ...
 Done. (0.379 sec)

 Estimated memory usage:
 Total:  296.21 MB
 orbitals            :   23.66 MB
 sparse matrices     :  173.00 MB
 global-size vectors :   10.77 MB
 spherical harmonics :   81.42 MB
 mixing histories    :    7.36 MB

 Finding rb for Na ...
 rb = {2.700 2.700 2.700}, int_b = -9.000387372942006, err_rb = 3.874e-04
 rb = {3.000 3.000 3.000}, int_b = -9.000387372942006, err_rb = 3.874e-04
 rb = {3.300 3.300 3.300}, int_b = -8.999937811172671, err_rb = 6.219e-05
 rb = {3.600 3.600 3.600}, int_b = -8.999999890359181, err_rb = 1.096e-07
```

```
rb = {3.600 3.600 3.600}
Finding rb for Cl ...
rb = {2.400 2.400 2.400}, int_b = -7.000203347008240, err_rb = 2.033e-04
rb = {2.700 2.700 2.700}, int_b = -7.000028751092675, err_rb = 2.875e-05
rb = {3.000 3.000 3.000}, int_b = -7.000028751092675, err_rb = 2.875e-05
rb = {3.300 3.300 3.300}, int_b = -7.000050803384491, err_rb = 5.080e-05
rb = {3.600 3.600 3.600}, int_b = -7.000029045901070, err_rb = 2.905e-05
rb = {3.900 3.900 3.900}, int_b = -7.000020121365980, err_rb = 2.012e-05
rb = {4.200 4.200 4.200}, int_b = -7.000020778263027, err_rb = 2.078e-05
rb = {4.500 4.500 4.500}, int_b = -7.000029043051562, err_rb = 2.904e-05
rb = {4.800 4.800 4.800}, int_b = -7.000037152188408, err_rb = 3.715e-05
rb = {5.100 5.100 5.100}, int_b = -7.000025996868315, err_rb = 2.600e-05
rb = {5.400 5.400 5.400}, int_b = -7.000032082424599, err_rb = 3.208e-05
rb = {5.700 5.700 5.700}, int_b = -7.000031540660014, err_rb = 3.154e-05
rb = {6.000 6.000 6.000}, int_b = -7.000033826871874, err_rb = 3.383e-05
rb = {6.300 6.300 6.300}, int_b = -6.999995536056760, err_rb = 4.464e-06
rb = {6.600 6.600 6.600}, int_b = -7.000000926125844, err_rb = 9.261e-07
rb = {6.900 6.900 6.900}, int_b = -6.999999819096163, err_rb = 1.809e-07
rb = {6.900 6.900 6.900}

################################################################
Relaxation step number: 1

Starting pseudocharge generation and self energy calculation...
WARNING: Atom 2 too close to boundary for b calculation
Integration b = 16.000000429934

Integration b_ref = 16.000000000001

**************************************
*          Eself_ref = 231.662318       *
**************************************
Done. (0.052285 s)
Time for b calculation: 0.077 seconds.

Starting calculating nonlocal projectors ...
Done. (0.039060 s)

~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
Starting SCF iteration...
AAR converged to a relative residual of 9.10138e-07 in 67 iterations.
Poisson problem took 0.827070s
==========================================
Relaxation iteration:  1
SCF iteration number:  1, Chebyshev cycle: 1
==========================================
Fermi energy = 2.351432
==========================================
Relaxation iteration:  1
SCF iteration number:  1, Chebyshev cycle: 2
==========================================
Fermi energy = 0.350625
==========================================
Relaxation iteration:  1
SCF iteration number:  1, Chebyshev cycle: 3
==========================================
Fermi energy = 0.081958
==========================================
Relaxation iteration:  1
SCF iteration number:  1, Chebyshev cycle: 4
==========================================
Fermi energy = 0.039456
------------------
Eband = -14.28341342
```

```
 Exc = -11.24389669
 Exc_dc = -12.78658909
 Eelec_dc = 25.50325668
 Eent = -0.00000001
 E_corr = 0.34194174
 Eself = 69.85015755
 Etot = -56.74568018
 ------------------
 Etot = -56.74568018
 Eatom = -28.37284009
 Error in SCF iteration: 1.1839e-01
 AAR converged to a relative residual of 6.69419e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 2.01572e-06 in 47 iterations.
 Poisson problem took 0.525329s
 This SCF iteration took 5.901 s.

 ========================
 Relaxation iteration:  1
 SCF iteration number:  2
 ========================
 Fermi energy = 0.012113
 ------------------
 Eband = -15.23435316
 Exc = -11.12247079
 Exc_dc = -12.62742059
 Eelec_dc = 26.56916768
 Eent = -0.00000001
 E_corr = 0.34194174
 Eself = 69.85015755
 Etot = -56.66845151
 ------------------
 Etot = -56.66845151
 Eatom = -28.33422575
 Error in SCF iteration: 7.3320e-02
 AAR converged to a relative residual of 4.56117e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 5.10992e-07 in 49 iterations.
 Poisson problem took 0.551418s
 This SCF iteration took 1.921 s.

 ========================
 Relaxation iteration:  1
 SCF iteration number:  3
 ========================
 Fermi energy = -0.010579
 ------------------
 Eband = -16.52447176
 Exc = -10.96833950
 Exc_dc = -12.42517938
 Eelec_dc = 27.97254467
 Eent = -0.00000001
 E_corr = 0.34194174
 Eself = 69.85015755
 Etot = -56.60330303
 ------------------
 Etot = -56.60330303
 Eatom = -28.30165152
 Error in SCF iteration: 3.4219e-02
 AAR converged to a relative residual of 5.87997e-05 in 19 iterations.
```

```
Density got negative

 AAR converged to a relative residual of 1.68979e-06 in 43 iterations.
 Poisson problem took 0.485728s
 This SCF iteration took 1.841 s.

 ========================
 Relaxation iteration:  1
 SCF iteration number:  4
 ========================
 Fermi energy = -0.026892
 ------------------
 Eband = -17.04814681
 Exc = -10.91227373
 Exc_dc = -12.35174470
 Eelec_dc = 28.52110722
 Eent = -0.00000001
 E_corr = 0.34194174
 Eself = 69.85015755
 Etot = -56.59578444
 ------------------
 Etot = -56.59578444
 Eatom = -28.29789222
 Error in SCF iteration: 1.6558e-02
 AAR converged to a relative residual of 5.75446e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 1.0517e-06 in 43 iterations.
 Poisson problem took 0.489622s
 This SCF iteration took 1.850 s.

 ========================
 Relaxation iteration:  1
 SCF iteration number:  5
 ========================
 Fermi energy = -0.037503
 ------------------
 Eband = -17.30941748
 Exc = -10.89072047
 Exc_dc = -12.32322600
 Eelec_dc = 28.79064847
 Eent = -0.00000001
 E_corr = 0.34194174
 Eself = 69.85015755
 Etot = -56.59447931
 ------------------
 Etot = -56.59447931
 Eatom = -28.29723965
 Error in SCF iteration: 5.7084e-03
 AAR converged to a relative residual of 5.64429e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 1.92905e-06 in 38 iterations.
 Poisson problem took 0.438785s
 This SCF iteration took 1.842 s.

 ========================
 Relaxation iteration:  1
 SCF iteration number:  6
 ========================
 Fermi energy = -0.038380
```

```
 ------------------
 Eband = -17.28521106
 Exc = -10.89995942
 Exc_dc = -12.33478127
 Eelec_dc = 28.76416928
 Eent = -0.00000001
 E_corr = 0.34194174
 Eself = 69.85015755
 Etot = -56.59443576
 ------------------
 Etot = -56.59443576
 Eatom = -28.29721788
 Error in SCF iteration: 1.2981e-03
 AAR converged to a relative residual of 6.20849e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 6.46483e-07 in 37 iterations.
 Poisson problem took 0.435245s
 This SCF iteration took 1.760 s.

 ========================
 Relaxation iteration:  1
 SCF iteration number:  7
 ========================
 Fermi energy = -0.039215
 ------------------
 Eband = -17.30069398
 Exc = -10.89940819
 Exc_dc = -12.33400278
 Eelec_dc = 28.77986763
 Eent = -0.00000001
 E_corr = 0.34194174
 Eself = 69.85015755
 Etot = -56.59444760
 ------------------
 Etot = -56.59444760
 Eatom = -28.29722380
 Error in SCF iteration: 6.6528e-04
 AAR converged to a relative residual of 7.45468e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 6.35751e-07 in 37 iterations.
 Poisson problem took 0.431079s
 This SCF iteration took 1.836 s.

 ========================
 Relaxation iteration:  1
 SCF iteration number:  8
 ========================
 Fermi energy = -0.039885
 ------------------
 Eband = -17.31499675
 Exc = -10.89880971
 Exc_dc = -12.33316177
 Eelec_dc = 28.79440324
 Eent = -0.00000001
 E_corr = 0.34194174
 Eself = 69.85015755
 Etot = -56.59445728
 ------------------
 Etot = -56.59445728
 Eatom = -28.29722864
```

```
 Error in SCF iteration: 2.9526e-04
 AAR converged to a relative residual of 7.80673e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 2.10986e-06 in 34 iterations.
 Poisson problem took 0.402416s
 This SCF iteration took 1.783 s.

 ========================
 Relaxation iteration:  1
 SCF iteration number:  9
 ========================
 Fermi energy = -0.040079
 ------------------
 Eband = -17.31762994
 Exc = -10.89867309
 Exc_dc = -12.33297168
 Eelec_dc = 28.79707354
 Eent = -0.00000001
 E_corr = 0.34194174
 Eself = 69.85015755
 Etot = -56.59447364
 ------------------
 Etot = -56.59447364
 Eatom = -28.29723682
 Error in SCF iteration: 1.0841e-04
 AAR converged to a relative residual of 8.1283e-05 in 21 iterations.

Density got negative

 AAR converged to a relative residual of 1.58552e-06 in 25 iterations.
 Poisson problem took 0.324865s
 This SCF iteration took 1.728 s.


 Finished SCF iteration in 9 steps!
 ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~

 ***********************************************************
 *          Energy per unit cell = -56.594473638 Ha.       *
 *          Energy per atom = -28.297236819 Ha.            *
 ***********************************************************

 Starting atomic force calculation ...
 WARNING: Atom 2 too close to boundary for b calculation
 local force calculation: 0.114 s
 ***********************************************************
 *                      Atomic Force                       *
 ***********************************************************
 Drift free forces (Ha/Bohr):
  -2.962471404609965  -0.000026605672629   0.000094308555448
   2.962471404609965   0.000026605672629  -0.000094308555448

 Max magnitude of forces (Ha/Bohr):   2.962471406230566


 Time for calculating forces: 0.215059 s.
 ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
 Final atomic positions (Cartesian) are as follows:
  5.000000       6.000000       6.000000
  7.000000       6.000000       6.000000

 Run-time of the program: 23.132149 seconds
```

```
rmpath(MSPARC_root);
rmpath(fullfile(MSPARC_root,"src"));
rmpath("M-SPARC\");
```

Here we choose kinetic energy cutoff in momentum space E_{cut} Ha for KSSOLV again.

```
Ecut2 = 20; % in Ha

% path and check
addpath(KSSOLV_root);
addpath("KSSOLV\");
KSSOLV_startup;
[K_mol2,K_Ham2,K_wf2,K_info2] = kssolv_diatomMol(atom1,atom2,L2,d,Ecut2);
```

```
The pseudopotential for Na is loaded from C:\Users\tvekua\OneDrive - MathWorks\Desktop\DFTMaterial\KSSOLV\/ppdata/de
The pseudopotential for Cl is loaded from C:\Users\tvekua\OneDrive - MathWorks\Desktop\DFTMaterial\KSSOLV\/ppdata/de
The pseudopotential for Na is loaded from C:\Users\tvekua\OneDrive - MathWorks\Desktop\DFTMaterial\KSSOLV\/ppdata/de
The pseudopotential for Cl is loaded from C:\Users\tvekua\OneDrive - MathWorks\Desktop\DFTMaterial\KSSOLV\/ppdata/de
Regular SCF for Pure DFT
Beging SCF calculation for □Í...
SCF iter   1:
eigtol =   1.000e-02
Rel Vtot Err    =            2.706e-01
Total Energy    = -4.6077794281887e+01
SCF iter   2:
eigtol =   1.000e-02
Rel Vtot Err    =            3.834e-02
Total Energy    = -4.7138689462095e+01
SCF iter   3:
eigtol =   4.793e-03
Rel Vtot Err    =            2.777e-02
Total Energy    = -4.7215731303151e+01
SCF iter   4:
eigtol =   3.471e-03
Rel Vtot Err    =            1.554e-03
Total Energy    = -4.7238307597986e+01
SCF iter   5:
eigtol =   1.942e-04
Rel Vtot Err    =            2.253e-04
Total Energy    = -4.7238320142749e+01
SCF iter   6:
eigtol =   2.816e-05
Rel Vtot Err    =            1.037e-05
Total Energy    = -4.7238320233109e+01
SCF iter   7:
eigtol =   1.296e-06
Rel Vtot Err    =            1.032e-06
Total Energy    = -4.7238320234276e+01
SCF iter   8:
eigtol =   1.290e-07
Rel Vtot Err    =            6.664e-08
Total Energy    = -4.7238320234284e+01
SCF iter   9:
eigtol =   8.329e-09
Rel Vtot Err    =            1.133e-08
Total Energy    = -4.7238320234284e+01
SCF iter  10:
eigtol =   1.417e-09
Rel Vtot Err    =            3.739e-09
Total Energy    = -4.7238320234284e+01
```

```
Convergence is reached!
resnrm =   1.370e-08
resnrm =   1.052e-08
resnrm =   4.777e-07
resnrm =   4.778e-07
---------------------
Elapsed time is 6.361084 seconds.
Etot            = -4.7238320234284e+01
Eone-electron   = -6.6494500616407e+01
Ehartree        =  2.3682086399281e+01
Exc             = -6.0614460905249e+00
Eewald          =  1.6355400733659e+00
Ealphat         =  0.0000000000000e+00
-------------------------------------
Total time used =            9.109e+00
||HX-XD||_F     =            6.758e-07
```

```
rmpath(KSSOLV_root);
rmpath("KSSOLV\");
fprintf("Total energy of diatomic (%s-%s) molecule from M-SPARC is %.6f Ha\n",
atom1, atom2, S2.Etotal);
```

```
Total energy of diatomic (Na-Cl) molecule from M-SPARC is -56.594474 Ha
```

```
fprintf("Atomic forces (Ha/Bohr) of diatomic (%s-%s) molecule from M-SPARC are \n
%10.6f %10.6f %10.6f\n %10.6f %10.6f %10.6f\n", atom1, atom2, S2.force');
```

```
Atomic forces (Ha/Bohr) of diatomic (Na-Cl) molecule from M-SPARC are
  -2.962471  -0.000027   0.000094
   2.962471   0.000027  -0.000094
```

```
fprintf("Total energy of diatomic (%s-%s) molecule from KSSOLV is %.6f Ha\n",
atom1, atom2, K_info2.Etot);
```

```
Total energy of diatomic (Na-Cl) molecule from KSSOLV is -47.238320 Ha
```

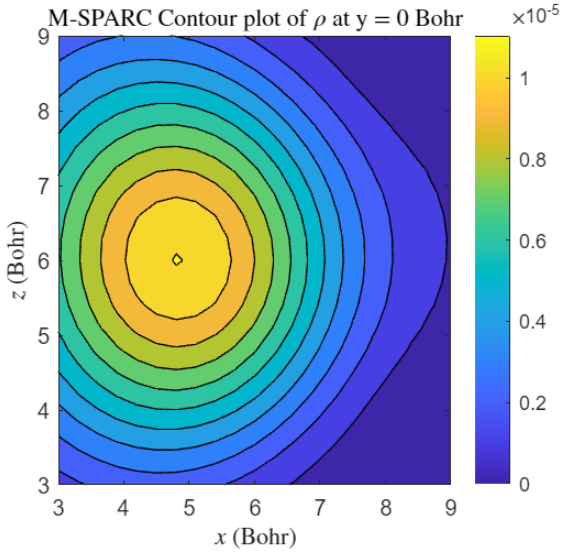
```
fprintf("Atomic forces (Ha/Bohr) of diatomic (%s-%s) molecule from KSSOLV are \n
%10.6f %10.6f %10.6f\n %10.6f %10.6f %10.6f\n", atom1, atom2, K_mol2.xyzforce');
```

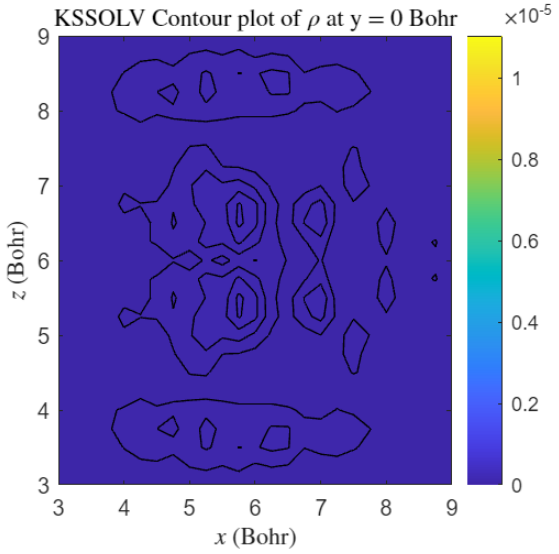
```
Atomic forces (Ha/Bohr) of diatomic (Na-Cl) molecule from KSSOLV are
  10.835215  -0.000000   0.000000
 -10.835240  -0.000000   0.000000
```

We visualize the contour plot of electron density from both solvers. We can choose the slice that we are interested to visualize below.

```
% M-SPARC
slice_allowed_m = string(linspace(0,S2.L2,S2.Ny));
zslicem = floor(double(slice_allowed_m(1))/S2.dy)+1; % in Bohr
x = linspace(0,L2,S2.Nx);
y = linspace(0,L2,S2.Ny);
z = linspace(0,L2,S2.Nz);
[X,~,Z] = ndgrid(x,y,z);
rhom = reshape(S2.rho(:,1),[S2.Nx S2.Ny S2.Nz]);
Xm = squeeze(X(:,zslicem,:));
Zm = squeeze(Z(:,zslicem,:));
rhom = squeeze(rhom(:,zslicem,:));
```

```
% KSSOLV
dyk = L2/K_Ham2.n2;
slice_allowed_k = string((0:dyk:L2));
zslicek = floor(double(slice_allowed_k(1))/dyk)+1; % in Bohr
x = linspace(0,L2,K_Ham2.n1);
y = linspace(0,L2,K_Ham2.n2);
z = linspace(0,L2,K_Ham2.n3);
[X,~,Z] = ndgrid(x,y,z);
Xk = squeeze(X(:,zslicek,:));
Yk = squeeze(Z(:,zslicek,:));
rhok = fftshift(K_Ham2.rho);
rhok = squeeze(rhok(:,zslicek,:));

fig2 = figure();
fig2.Position(3:4) = [1200, 450];
bottom = min(min(rhom(:)),min(rhok(:)));
top  = max(max(rhom(:)),max(rhok(:)));
subplot(1,2,1)
contourf(Xm,Zm,rhom)
shading interp;
colorbar
title("M-SPARC Contour plot of $\rho$ at y = "+ num2str((zslicem-1)*S2.dy,2) + "
Bohr", 'Interpreter','latex')
xlabel("$x$ (Bohr)",'Interpreter','latex')
ylabel("$z$ (Bohr)",'Interpreter','latex')
clim manual
clim([bottom top]);
xlim([(L2-3*d)/2 (L2+3*d)/2])
ylim([(L2-3*d)/2 (L2+3*d)/2])

subplot(1,2,2)
contourf(Xk,Yk,rhok)
shading interp;
colorbar
title("KSSOLV Contour plot of $\rho$ at y = "+ num2str((zslicek-1)*dyk,2) + "
Bohr", 'Interpreter','latex')
xlabel("$x$ (Bohr)",'Interpreter','latex')
ylabel("$z$ (Bohr)",'Interpreter','latex')
clim manual
clim([bottom top]);
colorbar;
xlim([(L2-3*d)/2 (L2+3*d)/2])
ylim([(L2-3*d)/2 (L2+3*d)/2])
```





Geometry Optimization

To find out the equlibrium bond length of the diatomic system, we can perform geometry optimization in both toolboxes. In M-SPARC, we need to turn on geomtry optimization by adding input option "RELAX_FLAG: 1".

```
addpath(MSPARC_root);
addpath(fullfile(MSPARC_root,"src"));
addpath("M-SPARC\");
% Real space toolbox M-SPARC
msparc_geoopt(atom1,atom2,L2,d,h2,MSPARC_root)
S3 = msparc("M-SPARC/geoopt");
```

```
 Reading .inpt file ...


<INPT>
# $ cat M-SPARC/geoopt.inpt
LATVEC_SCALE: 12.000000 12.000000 12.000000
MESH_SPACING: 0.300000
BC: D D D
EXCHANGE_CORRELATION: GGA_PBE
RELAX_FLAG: 1
<\INPT>

 Reading .ion file ...
 Number of atom types : 2
 Total number of atoms: 2
 Default atomic mass for Na is 22.989769
 Default atomic mass for Cl is 35.451500
 pseudo_dir # 1 = 11_Na_9_1.8_2.2_pbe_v1.0.psp8
 pseudo_dir # 2 = 17_Cl_7_1.9_1.9_pbe_n_v1.0.psp8

 COORD:
     5     6     6
     7     6     6

atom type 1, l = 0, r_core read 1.77096, change to rmax where |UdV| < 1E-8, 1.79000.
atom type 1, l = 1, r_core read 2.20971, change to rmax where |UdV| < 1E-8, 2.22000.
atom type 2, l = 0, r_core read 1.90538, change to rmax where |UdV| < 1E-8, 1.92000.
```

```
atom type 2, l = 1, r_core read 1.87149, change to rmax where |UdV| < 1E-8, 1.89000.
atom type 2, l = 2, r_core read 1.90538, change to rmax where |UdV| < 1E-8, 1.92000.
 reduced kpoint grid before symmetry:
     0     0     0

 reduced kpoint grid after symmetry:
     0     0     0

 nspin = 1, nspinor = 1, nspden = 1
## Chebyshev polynomial degree not provided, finding npl ...
## Based on the mesh size, npl is set to: 25
## Number of states not provided, finding Nev ...
## Based on the number of electrons, Nev is set to: 15
## Based on the desired accuracy, SCF_tol is set to: 2.989e-05
## Poisson tolerance not provided, choosing poisson_tol ...
## poisson_tol is set to: 2.989e-07
## Pseudocharge tolerance not provided, choosing pseudocharge_tol ...
## pseudocharge_tol is set to: 2.989e-08
 Creating differentiation matrices ...
 Done. (0.267 sec)

 Estimated memory usage:
 Total:  298.31 MB
 orbitals            :   23.66 MB
 sparse matrices     :  173.00 MB
 global-size vectors :   12.87 MB
 spherical harmonics :   81.42 MB
 mixing histories    :    7.36 MB

 Finding rb for Na ...
 rb = {2.700 2.700 2.700}, int_b = -9.000387372942006, err_rb = 3.874e-04
 rb = {3.000 3.000 3.000}, int_b = -9.000387372942006, err_rb = 3.874e-04
 rb = {3.300 3.300 3.300}, int_b = -8.999937811172671, err_rb = 6.219e-05
 rb = {3.600 3.600 3.600}, int_b = -8.999999890359181, err_rb = 1.096e-07
 rb = {3.900 3.900 3.900}, int_b = -8.999997579626214, err_rb = 2.420e-06
 rb = {4.200 4.200 4.200}, int_b = -8.999999654591255, err_rb = 3.454e-07
 rb = {4.500 4.500 4.500}, int_b = -9.000000026805850, err_rb = 2.681e-08
 rb = {4.500 4.500 4.500}
 Finding rb for Cl ...
 rb = {2.400 2.400 2.400}, int_b = -7.000203347008240, err_rb = 2.033e-04
 rb = {2.700 2.700 2.700}, int_b = -7.000028751092675, err_rb = 2.875e-05
 rb = {3.000 3.000 3.000}, int_b = -7.000028751092675, err_rb = 2.875e-05
 rb = {3.300 3.300 3.300}, int_b = -7.000050803384491, err_rb = 5.080e-05
 rb = {3.600 3.600 3.600}, int_b = -7.000029045901070, err_rb = 2.905e-05
 rb = {3.900 3.900 3.900}, int_b = -7.000020121365980, err_rb = 2.012e-05
 rb = {4.200 4.200 4.200}, int_b = -7.000020778263027, err_rb = 2.078e-05
 rb = {4.500 4.500 4.500}, int_b = -7.000029043051562, err_rb = 2.904e-05
 rb = {4.800 4.800 4.800}, int_b = -7.000037152188408, err_rb = 3.715e-05
 rb = {5.100 5.100 5.100}, int_b = -7.000025996868315, err_rb = 2.600e-05
 rb = {5.400 5.400 5.400}, int_b = -7.000032082424599, err_rb = 3.208e-05
 rb = {5.700 5.700 5.700}, int_b = -7.000031540660014, err_rb = 3.154e-05
 rb = {6.000 6.000 6.000}, int_b = -7.000033826871874, err_rb = 3.383e-05
 rb = {6.300 6.300 6.300}, int_b = -6.999995536056760, err_rb = 4.464e-06
 rb = {6.600 6.600 6.600}, int_b = -7.000000926125844, err_rb = 9.261e-07
 rb = {6.900 6.900 6.900}, int_b = -6.999999819096163, err_rb = 1.809e-07
 rb = {7.200 7.200 7.200}, int_b = -7.000000025313010, err_rb = 2.531e-08
 rb = {7.200 7.200 7.200}

 ###################################################################
 Relaxation step number: 1

 Starting pseudocharge generation and self energy calculation...
 WARNING: Atom 2 too close to boundary for b calculation
 Integration b = 16.000001656521
```

```
 Integration b_ref = 15.999999999995

 ***************************************
 *          Eself_ref = 231.662318       *
 ***************************************
 Done. (0.113026 s)
 Time for b calculation: 0.149 seconds.

 Starting calculating nonlocal projectors ...
 Done. (0.028533 s)

 ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
 Starting SCF iteration...
 AAR converged to a relative residual of 2.56122e-07 in 73 iterations.
 Poisson problem took 0.799014s
 ============================================
 Relaxation iteration:  1
 SCF iteration number:  1, Chebyshev cycle: 1
 ============================================
 Fermi energy = 2.351575
 ============================================
 Relaxation iteration:  1
 SCF iteration number:  1, Chebyshev cycle: 2
 ============================================
 Fermi energy = 0.349022
 ============================================
 Relaxation iteration:  1
 SCF iteration number:  1, Chebyshev cycle: 3
 ============================================
 Fermi energy = 0.081274
 ============================================
 Relaxation iteration:  1
 SCF iteration number:  1, Chebyshev cycle: 4
 ============================================
 Fermi energy = 0.039140
 ------------------
 Eband = -14.35827360
 Exc = -11.23418653
 Exc_dc = -12.77397457
 Eelec_dc = 25.58547690
 Eent = -0.00000004
 E_corr = 0.34194279
 Eself = 69.85015860
 Etot = -56.74122451
 ------------------
 Etot = -56.74122451
 Eatom = -28.37061226
 Error in SCF iteration: 1.1696e-01
 AAR converged to a relative residual of 6.65132e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 1.40665e-07 in 55 iterations.
 Poisson problem took 0.599735s
 This SCF iteration took 5.832 s.

 ========================
 Relaxation iteration:  1
 SCF iteration number:  2
 ========================
 Fermi energy = 0.012375
 ------------------
 Eband = -15.28294570
```

```
 Exc = -11.11658011
 Exc_dc = -12.61973225
 Eelec_dc = 26.62146697
 Eent = -0.00000004
 E_corr = 0.34194279
 Eself = 69.85015860
 Etot = -56.66654244
 ------------------
 Etot = -56.66654244
 Eatom = -28.33327122
 Error in SCF iteration: 7.2627e-02
 AAR converged to a relative residual of 4.53676e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 1.93265e-07 in 55 iterations.
 Poisson problem took 0.583157s
 This SCF iteration took 1.935 s.

 ========================
 Relaxation iteration:  1
 SCF iteration number:  3
 ========================
 Fermi energy = -0.009672
 ------------------
 Eband = -16.53920462
 Exc = -10.96710971
 Exc_dc = -12.42353179
 Eelec_dc = 27.98791121
 Eent = -0.00000004
 E_corr = 0.34194279
 Eself = 69.85015860
 Etot = -56.60308719
 ------------------
 Etot = -56.60308719
 Eatom = -28.30154360
 Error in SCF iteration: 3.3910e-02
 AAR converged to a relative residual of 5.84162e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 2.09759e-07 in 49 iterations.
 Poisson problem took 0.528141s
 This SCF iteration took 1.878 s.

 ========================
 Relaxation iteration:  1
 SCF iteration number:  4
 ========================
 Fermi energy = -0.025497
 ------------------
 Eband = -17.04578197
 Exc = -10.91278628
 Exc_dc = -12.35240048
 Eelec_dc = 28.51856346
 Eent = -0.00000004
 E_corr = 0.34194279
 Eself = 69.85015860
 Etot = -56.59582017
 ------------------
 Etot = -56.59582017
 Eatom = -28.29791008
 Error in SCF iteration: 1.6602e-02
 AAR converged to a relative residual of 5.6998e-05 in 19 iterations.
```

```
Density got negative

 AAR converged to a relative residual of 1.77549e-07 in 49 iterations.
 Poisson problem took 0.554475s
 This SCF iteration took 1.903 s.

 ========================
 Relaxation iteration:  1
 SCF iteration number:  5
 ========================
 Fermi energy = -0.036189
 ------------------
 Eband = -17.31172913
 Exc = -10.89055052
 Exc_dc = -12.32300539
 Eelec_dc = 28.79300704
 Eent = -0.00000004
 E_corr = 0.34194279
 Eself = 69.85015860
 Etot = -56.59448308
 ------------------
 Etot = -56.59448308
 Eatom = -28.29724154
 Error in SCF iteration: 5.7347e-03
 AAR converged to a relative residual of 5.63758e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 2.9564e-07 in 46 iterations.
 Poisson problem took 0.507631s
 This SCF iteration took 1.888 s.

 ========================
 Relaxation iteration:  1
 SCF iteration number:  6
 ========================
 Fermi energy = -0.037034
 ------------------
 Eband = -17.28584094
 Exc = -10.89997527
 Exc_dc = -12.33480253
 Eelec_dc = 28.76479283
 Eent = -0.00000004
 E_corr = 0.34194279
 Eself = 69.85015860
 Etot = -56.59443670
 ------------------
 Etot = -56.59443670
 Eatom = -28.29721835
 Error in SCF iteration: 1.2771e-03
 AAR converged to a relative residual of 6.02532e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 1.26158e-07 in 43 iterations.
 Poisson problem took 0.476961s
 This SCF iteration took 1.812 s.

 ========================
 Relaxation iteration:  1
 SCF iteration number:  7
 ========================
 Fermi energy = -0.037826
```

```
 ------------------
 Eband = -17.30039817
 Exc = -10.89944843
 Exc_dc = -12.33405908
 Eelec_dc = 28.77955612
 Eent = -0.00000004
 E_corr = 0.34194279
 Eself = 69.85015860
 Etot = -56.59444725
 ------------------
 Etot = -56.59444725
 Eatom = -28.29722362
 Error in SCF iteration: 6.7270e-04
 AAR converged to a relative residual of 7.43311e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 1.27184e-07 in 43 iterations.
 Poisson problem took 0.509657s
 This SCF iteration took 1.887 s.

 ========================
 Relaxation iteration:  1
 SCF iteration number:  8
 ========================
 Fermi energy = -0.038510
 ------------------
 Eband = -17.31494990
 Exc = -10.89883114
 Exc_dc = -12.33319130
 Eelec_dc = 28.79434855
 Eent = -0.00000004
 E_corr = 0.34194279
 Eself = 69.85015860
 Etot = -56.59445705
 ------------------
 Etot = -56.59445705
 Eatom = -28.29722852
 Error in SCF iteration: 2.8719e-04
 AAR converged to a relative residual of 7.68745e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 9.86702e-08 in 43 iterations.
 Poisson problem took 0.486923s
 This SCF iteration took 1.859 s.

 ========================
 Relaxation iteration:  1
 SCF iteration number:  9
 ========================
 Fermi energy = -0.038709
 ------------------
 Eband = -17.31772717
 Exc = -10.89868385
 Exc_dc = -12.33298654
 Eelec_dc = 28.79717234
 Eent = -0.00000004
 E_corr = 0.34194279
 Eself = 69.85015860
 Etot = -56.59446800
 ------------------
 Etot = -56.59446800
 Eatom = -28.29723400
```

```
 Error in SCF iteration: 1.0661e-04
 AAR converged to a relative residual of 8.08747e-05 in 21 iterations.

Density got negative

 AAR converged to a relative residual of 2.14298e-07 in 37 iterations.
 Poisson problem took 0.420212s
 This SCF iteration took 1.784 s.

 ========================
 Relaxation iteration:  1
 SCF iteration number: 10
 ========================
 Fermi energy = -0.038752
 ------------------
 Eband = -17.31839664
 Exc = -10.89868923
 Exc_dc = -12.33298901
 Eelec_dc = 28.79784234
 Eent = -0.00000004
 E_corr = 0.34194279
 Eself = 69.85015860
 Etot = -56.59447038
 ------------------
 Etot = -56.59447038
 Eatom = -28.29723519
 Error in SCF iteration: 6.8872e-05
 AAR converged to a relative residual of 6.88854e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 1.41682e-07 in 37 iterations.
 Poisson problem took 0.429310s
 This SCF iteration took 1.778 s.

 ========================
 Relaxation iteration:  1
 SCF iteration number: 11
 ========================
 Fermi energy = -0.038696
 ------------------
 Eband = -17.31745690
 Exc = -10.89872498
 Exc_dc = -12.33304156
 Eelec_dc = 28.79688522
 Eent = -0.00000004
 E_corr = 0.34194279
 Eself = 69.85015860
 Etot = -56.59447096
 ------------------
 Etot = -56.59447096
 Eatom = -28.29723548
 Error in SCF iteration: 2.6487e-05
 AAR converged to a relative residual of 7.05709e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 2.89909e-07 in 31 iterations.
 Poisson problem took 0.377794s
 This SCF iteration took 1.717 s.


 Finished SCF iteration in 11 steps!
 ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
```

```
*********************************************************
*          Energy per unit cell = -56.594470962 Ha.       *
*          Energy per atom = -28.297235481 Ha.            *
*********************************************************

Starting atomic force calculation ...
WARNING: Atom 2 too close to boundary for b calculation
local force calculation: 0.135 s
***********************************************************
*                      Atomic Force                       *
***********************************************************
Drift free forces (Ha/Bohr):
 -2.962972850521481  -0.000004092212288   0.000018830615446
  2.962972850521481   0.000004092212288  -0.000018830615446

Max magnitude of forces (Ha/Bohr):   2.962972850584145


Time for calculating forces: 0.250432 s.

Relaxation step number 1 completed in 25.606054 s.
~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~

######################################################################
Relaxation step number: 2

Starting pseudocharge generation and self energy calculation...
WARNING: Atom 2 too close to boundary for b calculation
Integration b = 16.000001902111

Integration b_ref = 15.999999999995

***************************************
*          Eself_ref = 231.653696       *
***************************************
Done. (0.049102 s)
Time for b calculation: 0.066 seconds.

Starting calculating nonlocal projectors ...
Done. (0.028407 s)

~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
Starting SCF iteration...
AAR converged to a relative residual of 2.58192e-07 in 74 iterations.
Poisson problem took 0.792714s
===========================================
Relaxation iteration:  2
SCF iteration number:  1, Chebyshev cycle: 1
===========================================
Fermi energy = -0.037984
------------------
Eband = -17.22723771
Exc = -10.89851392
Exc_dc = -12.33288217
Eelec_dc = 28.69495588
Eent = -0.00000005
E_corr = 0.33261008
Eself = 69.85018196
Etot = -56.61548551
------------------
Etot = -56.61548551
Eatom = -28.30774276
Error in SCF iteration: 7.0947e-03
```

```
 AAR converged to a relative residual of 5.06917e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 1.39703e-07 in 43 iterations.
 Poisson problem took 0.492687s
 This SCF iteration took 1.962 s.

 ========================
 Relaxation iteration:  2
 SCF iteration number:  2
 ========================
 Fermi energy = -0.038368
 ------------------
 Eband = -17.25594369
 Exc = -10.89559597
 Exc_dc = -12.32918770
 Eelec_dc = 28.72468875
 Eent = -0.00000005
 E_corr = 0.33261008
 Eself = 69.85018196
 Etot = -56.61523514
 ------------------
 Etot = -56.61523514
 Eatom = -28.30761757
 Error in SCF iteration: 4.1383e-03
 AAR converged to a relative residual of 3.49277e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 1.43037e-07 in 43 iterations.
 Poisson problem took 0.467676s
 This SCF iteration took 1.825 s.

 ========================
 Relaxation iteration:  2
 SCF iteration number:  3
 ========================
 Fermi energy = -0.038573
 ------------------
 Eband = -17.28472704
 Exc = -10.89325486
 Exc_dc = -12.32622770
 Eelec_dc = 28.75420658
 Eent = -0.00000005
 E_corr = 0.33261008
 Eself = 69.85018196
 Etot = -56.61511956
 ------------------
 Etot = -56.61511956
 Eatom = -28.30755978
 Error in SCF iteration: 1.1337e-03
 AAR converged to a relative residual of 4.40561e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 2.55585e-07 in 37 iterations.
 Poisson problem took 0.434161s
 This SCF iteration took 1.772 s.

 ========================
 Relaxation iteration:  2
 SCF iteration number:  4
 ========================
```

```
 Fermi energy = -0.038223
 ------------------
 Eband = -17.27769645
 Exc = -10.89475645
 Exc_dc = -12.32813779
 Eelec_dc = 28.74677423
 Eent = -0.00000005
 E_corr = 0.33261008
 Eself = 69.85018196
 Etot = -56.61511282
 ------------------
 Etot = -56.61511282
 Eatom = -28.30755641
 Error in SCF iteration: 2.8174e-04
 AAR converged to a relative residual of 3.96006e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 2.00461e-07 in 25 iterations.
 Poisson problem took 0.315121s
 This SCF iteration took 1.669 s.

 ========================
 Relaxation iteration:  2
 SCF iteration number:  5
 ========================
 Fermi energy = -0.038166
 ------------------
 Eband = -17.27565668
 Exc = -10.89493097
 Exc_dc = -12.32836582
 Eelec_dc = 28.74468137
 Eent = -0.00000005
 E_corr = 0.33261008
 Eself = 69.85018196
 Etot = -56.61511239
 ------------------
 Etot = -56.61511239
 Eatom = -28.30755620
 Error in SCF iteration: 8.3584e-05
 AAR converged to a relative residual of 4.68395e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 1.78485e-07 in 25 iterations.
 Poisson problem took 0.306905s
 This SCF iteration took 1.651 s.

 ========================
 Relaxation iteration:  2
 SCF iteration number:  6
 ========================
 Fermi energy = -0.038143
 ------------------
 Eband = -17.27508616
 Exc = -10.89496815
 Exc_dc = -12.32841528
 Eelec_dc = 28.74409822
 Eent = -0.00000005
 E_corr = 0.33261008
 Eself = 69.85018196
 Etot = -56.61511274
 ------------------
 Etot = -56.61511274
```

```
 Eatom = -28.30755637
 Error in SCF iteration: 4.9001e-05
 AAR converged to a relative residual of 6.59381e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 2.47623e-07 in 25 iterations.
 Poisson problem took 0.305242s
 This SCF iteration took 1.684 s.

 ========================
 Relaxation iteration:  2
 SCF iteration number:  7
 ========================
 Fermi energy = -0.038120
 ------------------
 Eband = -17.27472482
 Exc = -10.89497400
 Exc_dc = -12.32842470
 Eelec_dc = 28.74373365
 Eent = -0.00000005
 E_corr = 0.33261008
 Eself = 69.85018196
 Etot = -56.61511240
 ------------------
 Etot = -56.61511240
 Eatom = -28.30755620
 Error in SCF iteration: 1.6572e-05
 AAR converged to a relative residual of 6.46996e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 2.00477e-07 in 25 iterations.
 Poisson problem took 0.315121s
 This SCF iteration took 1.663 s.


 Finished SCF iteration in 7 steps!
 ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~

 ********************************************************
 *          Energy per unit cell = -56.615112403 Ha.       *
 *          Energy per atom = -28.307556202 Ha.            *
 ********************************************************

 Starting atomic force calculation ...
 WARNING: Atom 2 too close to boundary for b calculation
 local force calculation: 0.152 s
 ********************************************************
 *                      Atomic Force                    *
 ********************************************************
 Drift free forces (Ha/Bohr):
  -2.908772132725166  -0.000000237559667   0.000000672994516
   2.908772132725166   0.000000237559667  -0.000000672994516

 Max magnitude of forces (Ha/Bohr):   2.908772132725253


 Time for calculating forces: 0.249016 s.

 Relaxation step number 2 completed in 13.437515 s.
 ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~

 ################################################################
```

```
 Relaxation step number: 3

 Starting pseudocharge generation and self energy calculation...
 WARNING: Atom 2 too close to boundary for b calculation
 Integration b = 16.000002967097

 Integration b_ref = 15.999999999995

 ***************************************
 *          Eself_ref = 231.658388       *
 ***************************************
 Done. (0.041592 s)
 Time for b calculation: 0.061 seconds.

 Starting calculating nonlocal projectors ...
 Done. (0.007673 s)

 ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
 Starting SCF iteration...
 AAR converged to a relative residual of 2.90811e-07 in 73 iterations.
 Poisson problem took 0.801279s
 ===========================================
 Relaxation iteration:  3
 SCF iteration number:  1, Chebyshev cycle: 1
 ===========================================
 Fermi energy = -0.022158
 ------------------
 Eband = -15.27176359
 Exc = -10.89169002
 Exc_dc = -12.32536221
 Eelec_dc = 26.20536244
 Eent = -0.00000008
 E_corr = 0.15936139
 Eself = 69.85016991
 Etot = -57.32353756
 ------------------
 Etot = -57.32353756
 Eatom = -28.66176878
 Error in SCF iteration: 1.9418e-01
 AAR converged to a relative residual of 5.32845e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 2.91156e-07 in 59 iterations.
 Poisson problem took 0.628610s
 This SCF iteration took 2.081 s.

 ========================
 Relaxation iteration:  3
 SCF iteration number:  2
 ========================
 Fermi energy = -0.039225
 ------------------
 Eband = -15.88357482
 Exc = -10.81231912
 Exc_dc = -12.22425162
 Eelec_dc = 27.01994805
 Eent = -0.00000008
 E_corr = 0.15936139
 Eself = 69.85016991
 Etot = -57.14250286
 ------------------
 Etot = -57.14250286
 Eatom = -28.57125143
```

```
 Error in SCF iteration: 1.1173e-01
 AAR converged to a relative residual of 3.75643e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 2.77242e-07 in 55 iterations.
 Poisson problem took 0.607523s
 This SCF iteration took 1.938 s.

 ========================
 Relaxation iteration:  3
 SCF iteration number:  3
 ========================
 Fermi energy = -0.043460
 ------------------
 Eband = -16.48000426
 Exc = -10.76657583
 Exc_dc = -12.16645732
 Eelec_dc = 27.70842817
 Eent = -0.00000008
 E_corr = 0.15936139
 Eself = 69.85016991
 Etot = -57.06250318
 ------------------
 Etot = -57.06250318
 Eatom = -28.53125159
 Error in SCF iteration: 3.1868e-02
 AAR converged to a relative residual of 4.04794e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 2.11219e-07 in 49 iterations.
 Poisson problem took 0.535004s
 This SCF iteration took 1.874 s.

 ========================
 Relaxation iteration:  3
 SCF iteration number:  4
 ========================
 Fermi energy = -0.035539
 ------------------
 Eband = -16.25375725
 Exc = -10.81387705
 Exc_dc = -12.22668066
 Eelec_dc = 27.47371855
 Eent = -0.00000008
 E_corr = 0.15936139
 Eself = 69.85016991
 Etot = -57.05804368
 ------------------
 Etot = -57.05804368
 Eatom = -28.52902184
 Error in SCF iteration: 8.0840e-03
 AAR converged to a relative residual of 3.02019e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 2.28367e-07 in 43 iterations.
 Poisson problem took 0.474087s
 This SCF iteration took 1.800 s.

 ========================
 Relaxation iteration:  3
 SCF iteration number:  5
```

```
 ========================
 Fermi energy = -0.033847
 ------------------
 Eband = -16.20247007
 Exc = -10.82048554
 Exc_dc = -12.23521293
 Eelec_dc = 27.42063744
 Eent = -0.00000008
 E_corr = 0.15936139
 Eself = 69.85016991
 Etot = -57.05791383
 ------------------
 Etot = -57.05791383
 Eatom = -28.52895691
 Error in SCF iteration: 4.3612e-03
 AAR converged to a relative residual of 6.49319e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 2.6839e-07 in 43 iterations.
 Poisson problem took 0.485180s
 This SCF iteration took 1.815 s.

 ========================
 Relaxation iteration:  3
 SCF iteration number:  6
 ========================
 Fermi energy = -0.032465
 ------------------
 Eband = -16.16458091
 Exc = -10.82262646
 Exc_dc = -12.23812248
 Eelec_dc = 27.38201603
 Eent = -0.00000008
 E_corr = 0.15936139
 Eself = 69.85016991
 Etot = -57.05787745
 ------------------
 Etot = -57.05787745
 Eatom = -28.52893873
 Error in SCF iteration: 1.3824e-03
 AAR converged to a relative residual of 7.33373e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 1.77087e-07 in 43 iterations.
 Poisson problem took 0.508329s
 This SCF iteration took 1.888 s.

 ========================
 Relaxation iteration:  3
 SCF iteration number:  7
 ========================
 Fermi energy = -0.031645
 ------------------
 Eband = -16.15000934
 Exc = -10.82328785
 Exc_dc = -12.23901222
 Eelec_dc = 27.36718966
 Eent = -0.00000008
 E_corr = 0.15936139
 Eself = 69.85016991
 Etot = -57.05790390
 ------------------
```

```
 Etot = -57.05790390
 Eatom = -28.52895195
 Error in SCF iteration: 5.2781e-04
 AAR converged to a relative residual of 7.72839e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 2.72154e-07 in 37 iterations.
 Poisson problem took 0.423776s
 This SCF iteration took 1.738 s.

 ========================
 Relaxation iteration:  3
 SCF iteration number:  8
 ========================
 Fermi energy = -0.031591
 ------------------
 Eband = -16.14770403
 Exc = -10.82318135
 Exc_dc = -12.23888451
 Eelec_dc = 27.36489460
 Eent = -0.00000008
 E_corr = 0.15936139
 Eself = 69.85016991
 Etot = -57.05791487
 ------------------
 Etot = -57.05791487
 Eatom = -28.52895744
 Error in SCF iteration: 3.4638e-04
 AAR converged to a relative residual of 3.67904e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 1.08333e-07 in 43 iterations.
 Poisson problem took 0.472275s
 This SCF iteration took 1.846 s.

 ========================
 Relaxation iteration:  3
 SCF iteration number:  9
 ========================
 Fermi energy = -0.031397
 ------------------
 Eband = -16.14185330
 Exc = -10.82347572
 Exc_dc = -12.23925124
 Eelec_dc = 27.35895552
 Eent = -0.00000008
 E_corr = 0.15936139
 Eself = 69.85016991
 Etot = -57.05793085
 ------------------
 Etot = -57.05793085
 Eatom = -28.52896543
 Error in SCF iteration: 1.1244e-04
 AAR converged to a relative residual of 3.69725e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 1.33062e-07 in 37 iterations.
 Poisson problem took 0.421527s
 This SCF iteration took 1.752 s.

 ========================
```

```
 Relaxation iteration:  3
 SCF iteration number: 10
 ========================
 Fermi energy = -0.031486
 ------------------
 Eband = -16.14335319
 Exc = -10.82326921
 Exc_dc = -12.23897565
 Eelec_dc = 27.36051921
 Eent = -0.00000008
 E_corr = 0.15936139
 Eself = 69.85016991
 Etot = -57.05793614
 ------------------
 Etot = -57.05793614
 Eatom = -28.52896807
 Error in SCF iteration: 4.8759e-05
 AAR converged to a relative residual of 5.16561e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 1.4903e-07 in 31 iterations.
 Poisson problem took 0.368879s
 This SCF iteration took 1.747 s.

 ========================
 Relaxation iteration:  3
 SCF iteration number: 11
 ========================
 Fermi energy = -0.031509
 ------------------
 Eband = -16.14388150
 Exc = -10.82320078
 Exc_dc = -12.23888567
 Eelec_dc = 27.36106796
 Eent = -0.00000008
 E_corr = 0.15936139
 Eself = 69.85016991
 Etot = -57.05793725
 ------------------
 Etot = -57.05793725
 Eatom = -28.52896863
 Error in SCF iteration: 2.7310e-05
 AAR converged to a relative residual of 6.34002e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 2.26091e-07 in 19 iterations.
 Poisson problem took 0.251973s
 This SCF iteration took 1.570 s.


 Finished SCF iteration in 11 steps!
 ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~

 ********************************************************
 *          Energy per unit cell = -57.057937251 Ha.       *
 *          Energy per atom = -28.528968626 Ha.            *
 ********************************************************

 Starting atomic force calculation ...
 WARNING: Atom 2 too close to boundary for b calculation
 local force calculation: 0.089 s
 ********************************************************
```

```
*                      Atomic Force                       *
***********************************************************
Drift free forces (Ha/Bohr):
 -1.861944775492895  -0.000000031491653   0.000000059680449
  1.861944775492895   0.000000031491653  -0.000000059680449

Max magnitude of forces (Ha/Bohr):   1.861944775492897


Time for calculating forces: 0.194864 s.

Relaxation step number 3 completed in 21.220279 s.
~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~

#####################################################################
Relaxation step number: 4

Starting pseudocharge generation and self energy calculation...
WARNING: Atom 2 too close to boundary for b calculation
Integration b = 16.000002567825

Integration b_ref = 15.999999999995

***************************************
*          Eself_ref = 231.810893       *
***************************************
Done. (0.033387 s)
Time for b calculation: 0.047 seconds.

Starting calculating nonlocal projectors ...
Done. (0.005375 s)

~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
Starting SCF iteration...
AAR converged to a relative residual of 2.80481e-07 in 73 iterations.
Poisson problem took 0.789426s
===========================================
Relaxation iteration:  4
SCF iteration number:  1, Chebyshev cycle: 1
===========================================
Fermi energy = -0.038254
------------------
Eband = -14.86383336
Exc = -10.75985398
Exc_dc = -12.15599090
Eelec_dc = 25.77980981
Eent = -0.00000007
E_corr = 0.05465004
Eself = 69.84972222
Etot = -57.48295886
------------------
Etot = -57.48295886
Eatom = -28.74147943
Error in SCF iteration: 2.1725e-02
AAR converged to a relative residual of 3.3726e-05 in 19 iterations.

Density got negative

AAR converged to a relative residual of 2.84749e-07 in 48 iterations.
Poisson problem took 0.520876s
This SCF iteration took 2.027 s.

========================
Relaxation iteration:  4
```

```
 SCF iteration number:  2
 ========================
 Fermi energy = -0.036921
 ------------------
 Eband = -14.74651681
 Exc = -10.77679460
 Exc_dc = -12.17742273
 Eelec_dc = 25.65886125
 Eent = -0.00000007
 E_corr = 0.05465004
 Eself = 69.84972222
 Etot = -57.48209968
 ------------------
 Etot = -57.48209968
 Eatom = -28.74104984
 Error in SCF iteration: 1.2814e-02
 AAR converged to a relative residual of 2.52093e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 7.46329e-08 in 49 iterations.
 Poisson problem took 0.553455s
 This SCF iteration took 1.894 s.

 ========================
 Relaxation iteration:  4
 SCF iteration number:  3
 ========================
 Fermi energy = -0.033359
 ------------------
 Eband = -14.61246750
 Exc = -10.79624244
 Exc_dc = -12.20209152
 Eelec_dc = 25.51989758
 Eent = -0.00000007
 E_corr = 0.05465004
 Eself = 69.84972222
 Etot = -57.48179310
 ------------------
 Etot = -57.48179310
 Eatom = -28.74089655
 Error in SCF iteration: 4.1279e-03
 AAR converged to a relative residual of 2.14494e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 1.68957e-07 in 43 iterations.
 Poisson problem took 0.480835s
 This SCF iteration took 1.812 s.

 ========================
 Relaxation iteration:  4
 SCF iteration number:  4
 ========================
 Fermi energy = -0.032962
 ------------------
 Eband = -14.61933434
 Exc = -10.79422585
 Exc_dc = -12.19965503
 Eelec_dc = 25.52705751
 Eent = -0.00000007
 E_corr = 0.05465004
 Eself = 69.84972222
 Etot = -57.48191990
```

```
 ------------------
 Etot = -57.48191990
 Eatom = -28.74095995
 Error in SCF iteration: 1.4125e-03
 AAR converged to a relative residual of 4.787e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 2.9149e-07 in 39 iterations.
 Poisson problem took 0.472336s
 This SCF iteration took 1.838 s.

 ========================
 Relaxation iteration:  4
 SCF iteration number:  5
 ========================
 Fermi energy = -0.032746
 ------------------
 Eband = -14.61940798
 Exc = -10.79377834
 Exc_dc = -12.19914842
 Eelec_dc = 25.52717231
 Eent = -0.00000007
 E_corr = 0.05465004
 Eself = 69.84972222
 Etot = -57.48193783
 ------------------
 Etot = -57.48193783
 Eatom = -28.74096892
 Error in SCF iteration: 5.1905e-04
 AAR converged to a relative residual of 6.37405e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 2.8142e-07 in 41 iterations.
 Poisson problem took 0.459186s
 This SCF iteration took 1.823 s.

 ========================
 Relaxation iteration:  4
 SCF iteration number:  6
 ========================
 Fermi energy = -0.032596
 ------------------
 Eband = -14.61859786
 Exc = -10.79351508
 Exc_dc = -12.19877561
 Eelec_dc = 25.52645673
 Eent = -0.00000007
 E_corr = 0.05465004
 Eself = 69.84972222
 Etot = -57.48195285
 ------------------
 Etot = -57.48195285
 Eatom = -28.74097643
 Error in SCF iteration: 2.2462e-04
 AAR converged to a relative residual of 5.75601e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 2.19284e-07 in 37 iterations.
 Poisson problem took 0.415477s
 This SCF iteration took 1.769 s.
```

```
 ========================
 Relaxation iteration:  4
 SCF iteration number:  7
 ========================
 Fermi energy = -0.032570
 ------------------
 Eband = -14.61906477
 Exc = -10.79327597
 Exc_dc = -12.19845979
 Eelec_dc = 25.52699319
 Eent = -0.00000007
 E_corr = 0.05465004
 Eself = 69.84972222
 Etot = -57.48196000
 ------------------
 Etot = -57.48196000
 Eatom = -28.74098000
 Error in SCF iteration: 1.3130e-04
 AAR converged to a relative residual of 7.4503e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 1.34195e-07 in 31 iterations.
 Poisson problem took 0.361942s
 This SCF iteration took 1.680 s.

 ========================
 Relaxation iteration:  4
 SCF iteration number:  8
 ========================
 Fermi energy = -0.032578
 ------------------
 Eband = -14.61959573
 Exc = -10.79311269
 Exc_dc = -12.19823522
 Eelec_dc = 25.52757982
 Eent = -0.00000007
 E_corr = 0.05465004
 Eself = 69.84972222
 Etot = -57.48196562
 ------------------
 Etot = -57.48196562
 Eatom = -28.74098281
 Error in SCF iteration: 6.0867e-05
 AAR converged to a relative residual of 2.95737e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 1.07258e-07 in 37 iterations.
 Poisson problem took 0.443654s
 This SCF iteration took 1.802 s.

 ========================
 Relaxation iteration:  4
 SCF iteration number:  9
 ========================
 Fermi energy = -0.032584
 ------------------
 Eband = -14.62009874
 Exc = -10.79305150
 Exc_dc = -12.19814317
 Eelec_dc = 25.52811048
 Eent = -0.00000007
 E_corr = 0.05465004
```

```
 Eself = 69.84972222
 Etot = -57.48196883
 ------------------
 Etot = -57.48196883
 Eatom = -28.74098441
 Error in SCF iteration: 2.1608e-05
 AAR converged to a relative residual of 2.52234e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 2.28524e-07 in 25 iterations.
 Poisson problem took 0.316531s
 This SCF iteration took 1.665 s.


 Finished SCF iteration in 9 steps!
 ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~

 ********************************************************
 *          Energy per unit cell = -57.481968828 Ha.       *
 *          Energy per atom = -28.740984414 Ha.            *
 ********************************************************

 Starting atomic force calculation ...
 WARNING: Atom 2 too close to boundary for b calculation
 local force calculation: 0.086 s
 ************************************************************
 *                      Atomic Force                        *
 ************************************************************
 Drift free forces (Ha/Bohr):
  -1.217776821984487  -0.000000054015563  -0.000000034182327
   1.217776821984487   0.000000054015563   0.000000034182327

 Max magnitude of forces (Ha/Bohr):   1.217776821984489


 Time for calculating forces: 0.192203 s.

 Relaxation step number 4 completed in 17.418953 s.
 ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~

 ######################################################################
 Relaxation step number: 5

 Starting pseudocharge generation and self energy calculation...
 WARNING: Atom 2 too close to boundary for b calculation
 Integration b = 16.000002250301

 Integration b_ref = 15.999999999995

 ************************************
 *          Eself_ref = 231.609072       *
 ************************************
 Done. (0.032480 s)
 Time for b calculation: 0.044 seconds.

 Starting calculating nonlocal projectors ...
 Done. (0.004688 s)

 ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
 Starting SCF iteration...
 AAR converged to a relative residual of 2.93882e-07 in 76 iterations.
 Poisson problem took 0.834173s
 ===========================================
```

```
 Relaxation iteration:  5
 SCF iteration number:  1, Chebyshev cycle: 1
 ============================================
 Fermi energy = -0.031636
 ------------------
 Eband = -13.51570410
 Exc = -10.80533676
 Exc_dc = -12.21308316
 Eelec_dc = 24.18305903
 Eent = -0.00000006
 E_corr = 0.01912639
 Eself = 69.85029972
 Etot = -57.75607205
 ------------------
 Etot = -57.75607205
 Eatom = -28.87803603
 Error in SCF iteration: 1.1705e-02
 AAR converged to a relative residual of 1.51445e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 1.63491e-07 in 43 iterations.
 Poisson problem took 0.470577s
 This SCF iteration took 1.973 s.

 ========================
 Relaxation iteration:  5
 SCF iteration number:  2
 ========================
 Fermi energy = -0.033104
 ------------------
 Eband = -13.56287208
 Exc = -10.79600110
 Exc_dc = -12.20063680
 Eelec_dc = 24.23268103
 Eent = -0.00000006
 E_corr = 0.01912639
 Eself = 69.85029972
 Etot = -57.75672874
 ------------------
 Etot = -57.75672874
 Eatom = -28.87836437
 Error in SCF iteration: 8.0246e-03
 AAR converged to a relative residual of 2.04874e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 2.66556e-07 in 44 iterations.
 Poisson problem took 0.495614s
 This SCF iteration took 1.833 s.

 ========================
 Relaxation iteration:  5
 SCF iteration number:  3
 ========================
 Fermi energy = -0.032679
 ------------------
 Eband = -13.65700554
 Exc = -10.77883965
 Exc_dc = -12.17754959
 Eelec_dc = 24.33259429
 Eent = -0.00000006
 E_corr = 0.01912639
 Eself = 69.85029972
```

```
 Etot = -57.75687470
 ------------------
 Etot = -57.75687470
 Eatom = -28.87843735
 Error in SCF iteration: 1.9560e-03
 AAR converged to a relative residual of 2.97438e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 2.91872e-07 in 41 iterations.
 Poisson problem took 0.456116s
 This SCF iteration took 1.834 s.

 ========================
 Relaxation iteration:  5
 SCF iteration number:  4
 ========================
 Fermi energy = -0.033047
 ------------------
 Eband = -13.66352296
 Exc = -10.77853618
 Exc_dc = -12.17697348
 Eelec_dc = 24.33934639
 Eent = -0.00000006
 E_corr = 0.01912639
 Eself = 69.85029972
 Etot = -57.75691266
 ------------------
 Etot = -57.75691266
 Eatom = -28.87845633
 Error in SCF iteration: 9.3297e-04
 AAR converged to a relative residual of 8.33927e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 2.83171e-07 in 41 iterations.
 Poisson problem took 0.459959s
 This SCF iteration took 1.806 s.

 ========================
 Relaxation iteration:  5
 SCF iteration number:  5
 ========================
 Fermi energy = -0.033398
 ------------------
 Eband = -13.66633477
 Exc = -10.77893679
 Exc_dc = -12.17738352
 Eelec_dc = 24.34214311
 Eent = -0.00000006
 E_corr = 0.01912639
 Eself = 69.85029972
 Etot = -57.75691832
 ------------------
 Etot = -57.75691832
 Eatom = -28.87845916
 Error in SCF iteration: 2.4059e-04
 AAR converged to a relative residual of 8.66999e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 2.19216e-07 in 37 iterations.
 Poisson problem took 0.420499s
 This SCF iteration took 1.799 s.
```

```
 ========================
 Relaxation iteration:  5
 SCF iteration number:  6
 ========================
 Fermi energy = -0.033606
 ------------------
 Eband = -13.67060118
 Exc = -10.77858277
 Exc_dc = -12.17692044
 Eelec_dc = 24.34651623
 Eent = -0.00000006
 E_corr = 0.01912639
 Eself = 69.85029972
 Etot = -57.75692068
 ------------------
 Etot = -57.75692068
 Eatom = -28.87846034
 Error in SCF iteration: 1.2846e-04
 AAR converged to a relative residual of 6.26981e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 2.2249e-07 in 37 iterations.
 Poisson problem took 0.421719s
 This SCF iteration took 1.741 s.

 ========================
 Relaxation iteration:  5
 SCF iteration number:  7
 ========================
 Fermi energy = -0.033781
 ------------------
 Eband = -13.67390337
 Exc = -10.77828251
 Exc_dc = -12.17652296
 Eelec_dc = 24.34991292
 Eent = -0.00000006
 E_corr = 0.01912639
 Eself = 69.85029972
 Etot = -57.75692339
 ------------------
 Etot = -57.75692339
 Eatom = -28.87846169
 Error in SCF iteration: 6.2564e-05
 AAR converged to a relative residual of 5.17895e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 9.98381e-08 in 37 iterations.
 Poisson problem took 0.417607s
 This SCF iteration took 1.790 s.

 ========================
 Relaxation iteration:  5
 SCF iteration number:  8
 ========================
 Fermi energy = -0.033835
 ------------------
 Eband = -13.67423787
 Exc = -10.77831820
 Exc_dc = -12.17656809
 Eelec_dc = 24.35023729
 Eent = -0.00000006
```

```
 E_corr = 0.01912639
 Eself = 69.85029972
 Etot = -57.75692408
 ------------------
 Etot = -57.75692408
 Eatom = -28.87846204
 Error in SCF iteration: 3.0447e-05
 AAR converged to a relative residual of 4.26387e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 2.78259e-07 in 26 iterations.
 Poisson problem took 0.316290s
 This SCF iteration took 1.646 s.

 ========================
 Relaxation iteration:  5
 SCF iteration number:  9
 ========================
 Fermi energy = -0.033859
 ------------------
 Eband = -13.67408319
 Exc = -10.77835796
 Exc_dc = -12.17662228
 Eelec_dc = 24.35006725
 Eent = -0.00000006
 E_corr = 0.01912639
 Eself = 69.85029972
 Etot = -57.75692501
 ------------------
 Etot = -57.75692501
 Eatom = -28.87846251
 Error in SCF iteration: 1.0101e-05
 AAR converged to a relative residual of 6.07278e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 2.05083e-07 in 19 iterations.
 Poisson problem took 0.261599s
 This SCF iteration took 1.641 s.


 Finished SCF iteration in 9 steps!
 ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~

 ***********************************************************
 *          Energy per unit cell = -57.756925015 Ha.       *
 *          Energy per atom = -28.878462507 Ha.            *
 ***********************************************************

 Starting atomic force calculation ...
 WARNING: Atom 2 too close to boundary for b calculation
 local force calculation: 0.083 s
 ***********************************************************
 *                      Atomic Force                       *
 ***********************************************************
 Drift free forces (Ha/Bohr):
  -0.853384909427527  -0.000000011129324   0.000000042619800
   0.853384909427527   0.000000011129324  -0.000000042619800

 Max magnitude of forces (Ha/Bohr):   0.853384909427528


 Time for calculating forces: 0.176586 s.
```

```
 Relaxation step number 5 completed in 17.196979 s.
 ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~

 ######################################################################
 Relaxation step number: 6

 Starting pseudocharge generation and self energy calculation...
 WARNING: Atom 1 too close to boundary for b calculation
 WARNING: Atom 2 too close to boundary for b calculation
 Integration b = 16.000003000244

 Integration b_ref = 15.999999999995

 ************************************
 *          Eself_ref = 231.841592       *
 ************************************
 Done. (0.032099 s)
 Time for b calculation: 0.046 seconds.

 Starting calculating nonlocal projectors ...
 Done. (0.007048 s)

 ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
 Starting SCF iteration...
 AAR converged to a relative residual of 1.13183e-07 in 79 iterations.
 Poisson problem took 0.829180s
 ===========================================
 Relaxation iteration:  6
 SCF iteration number:  1, Chebyshev cycle: 1
 ===========================================
 Fermi energy = -0.011001
 ------------------
 Eband = -12.76195926
 Exc = -10.81349998
 Exc_dc = -12.22293147
 Eelec_dc = 23.24654085
 Eent = -0.00000008
 E_corr = 0.00531491
 Eself = 69.84961725
 Etot = -57.95028934
 ------------------
 Etot = -57.95028934
 Eatom = -28.97514467
 Error in SCF iteration: 2.2615e-02
 AAR converged to a relative residual of 1.74289e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 2.97956e-07 in 43 iterations.
 Poisson problem took 0.513092s
 This SCF iteration took 1.966 s.

 ========================
 Relaxation iteration:  6
 SCF iteration number:  2
 ========================
 Fermi energy = -0.020057
 ------------------
 Eband = -12.88526056
 Exc = -10.79097927
 Exc_dc = -12.19328265
 Eelec_dc = 23.37588246
 Eent = -0.00000008
```

```
 E_corr = 0.00531491
 Eself = 69.84961725
 Etot = -57.95137714
 ------------------
 Etot = -57.95137714
 Eatom = -28.97568857
 Error in SCF iteration: 1.5632e-02
 AAR converged to a relative residual of 3.28127e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 2.39181e-07 in 49 iterations.
 Poisson problem took 0.555151s
 This SCF iteration took 1.875 s.

 ========================
 Relaxation iteration:  6
 SCF iteration number:  3
 ========================
 Fermi energy = -0.027518
 ------------------
 Eband = -13.14450239
 Exc = -10.74631647
 Exc_dc = -12.13423633
 Eelec_dc = 23.64929673
 Eent = -0.00000008
 E_corr = 0.00531491
 Eself = 69.84961725
 Etot = -57.95158822
 ------------------
 Etot = -57.95158822
 Eatom = -28.97579411
 Error in SCF iteration: 4.4465e-03
 AAR converged to a relative residual of 3.18764e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 1.57786e-07 in 43 iterations.
 Poisson problem took 0.569922s
 This SCF iteration took 2.007 s.

 ========================
 Relaxation iteration:  6
 SCF iteration number:  4
 ========================
 Fermi energy = -0.030103
 ------------------
 Eband = -13.16162560
 Exc = -10.74534573
 Exc_dc = -12.13261765
 Eelec_dc = 23.66693495
 Eent = -0.00000008
 E_corr = 0.00531491
 Eself = 69.84961725
 Etot = -57.95172115
 ------------------
 Etot = -57.95172115
 Eatom = -28.97586057
 Error in SCF iteration: 2.1778e-03
 AAR converged to a relative residual of 7.93198e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 1.72557e-07 in 43 iterations.
```

```
 Poisson problem took 0.526739s
 This SCF iteration took 1.948 s.

 ========================
 Relaxation iteration:  6
 SCF iteration number:  5
 ========================
 Fermi energy = -0.032038
 ------------------
 Eband = -13.18438172
 Exc = -10.74350508
 Exc_dc = -12.12989910
 Eelec_dc = 23.69051427
 Eent = -0.00000008
 E_corr = 0.00531491
 Eself = 69.84961725
 Etot = -57.95177585
 ------------------
 Etot = -57.95177585
 Eatom = -28.97588792
 Error in SCF iteration: 6.0974e-04
 AAR converged to a relative residual of 6.93565e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 1.1059e-07 in 43 iterations.
 Poisson problem took 0.479417s
 This SCF iteration took 1.877 s.

 ========================
 Relaxation iteration:  6
 SCF iteration number:  6
 ========================
 Fermi energy = -0.033407
 ------------------
 Eband = -13.19773839
 Exc = -10.74231853
 Exc_dc = -12.12828433
 Eelec_dc = 23.70425613
 Eent = -0.00000008
 E_corr = 0.00531491
 Eself = 69.84961725
 Etot = -57.95181889
 ------------------
 Etot = -57.95181889
 Eatom = -28.97590944
 Error in SCF iteration: 2.5209e-04
 AAR converged to a relative residual of 5.99765e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 2.95301e-07 in 38 iterations.
 Poisson problem took 0.421930s
 This SCF iteration took 1.759 s.

 ========================
 Relaxation iteration:  6
 SCF iteration number:  7
 ========================
 Fermi energy = -0.033880
 ------------------
 Eband = -13.20161014
 Exc = -10.74194475
 Exc_dc = -12.12777353
```

```
 Eelec_dc = 23.70825044
 Eent = -0.00000008
 E_corr = 0.00531491
 Eself = 69.84961725
 Etot = -57.95183335
 ------------------
 Etot = -57.95183335
 Eatom = -28.97591668
 Error in SCF iteration: 1.6276e-04
 AAR converged to a relative residual of 8.18076e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 1.7707e-07 in 37 iterations.
 Poisson problem took 0.419161s
 This SCF iteration took 1.794 s.

 ========================
 Relaxation iteration:  6
 SCF iteration number:  8
 ========================
 Fermi energy = -0.034217
 ------------------
 Eband = -13.20063040
 Exc = -10.74212995
 Exc_dc = -12.12800980
 Eelec_dc = 23.70720932
 Eent = -0.00000008
 E_corr = 0.00531491
 Eself = 69.84961725
 Etot = -57.95184365
 ------------------
 Etot = -57.95184365
 Eatom = -28.97592182
 Error in SCF iteration: 7.6073e-05
 AAR converged to a relative residual of 6.58817e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 2.98336e-07 in 33 iterations.
 Poisson problem took 0.378763s
 This SCF iteration took 1.711 s.

 ========================
 Relaxation iteration:  6
 SCF iteration number:  9
 ========================
 Fermi energy = -0.034408
 ------------------
 Eband = -13.20091455
 Exc = -10.74206708
 Exc_dc = -12.12793381
 Eelec_dc = 23.70750196
 Eent = -0.00000008
 E_corr = 0.00531491
 Eself = 69.84961725
 Etot = -57.95184829
 ------------------
 Etot = -57.95184829
 Eatom = -28.97592414
 Error in SCF iteration: 2.5757e-05
 AAR converged to a relative residual of 5.35255e-05 in 19 iterations.

Density got negative
```

```
AAR converged to a relative residual of 1.58591e-07 in 25 iterations.
Poisson problem took 0.311250s
This SCF iteration took 1.712 s.


Finished SCF iteration in 9 steps!
~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~

*********************************************************
*          Energy per unit cell = -57.951848290 Ha.       *
*          Energy per atom = -28.975924145 Ha.            *
*********************************************************

Starting atomic force calculation ...
WARNING: Atom 2 too close to boundary for b calculation
local force calculation: 0.086 s
*********************************************************
*                      Atomic Force                     *
*********************************************************
Drift free forces (Ha/Bohr):
 -0.534801026293761  -0.000000003041952   0.000000028083248
  0.534801026293761   0.000000003041952  -0.000000028083248

Max magnitude of forces (Ha/Bohr):   0.534801026293762


Time for calculating forces: 0.176687 s.

Relaxation step number 6 completed in 17.779354 s.
~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~

######################################################################
Relaxation step number: 7

Starting pseudocharge generation and self energy calculation...
WARNING: Atom 1 too close to boundary for b calculation
WARNING: Atom 2 too close to boundary for b calculation
Integration b = 16.000002568531

Integration b_ref = 15.999999999995

***************************************
*          Eself_ref = 231.600453       *
***************************************
Done. (0.033829 s)
Time for b calculation: 0.047 seconds.

Starting calculating nonlocal projectors ...
Done. (0.005238 s)

~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
Starting SCF iteration...
AAR converged to a relative residual of 2.8901e-07 in 77 iterations.
Poisson problem took 0.808718s
==========================================
Relaxation iteration:  7
SCF iteration number:  1, Chebyshev cycle: 1
==========================================
Fermi energy = -0.032995
------------------
Eband = -12.96613681
Exc = -10.71493170
Exc_dc = -12.09255261
```

```
 Eelec_dc = 23.38433191
 Eent = -0.00000007
 E_corr = 0.00145896
 Eself = 69.85032208
 Etot = -58.05304717
 ------------------
 Etot = -58.05304717
 Eatom = -29.02652359
 Error in SCF iteration: 5.8119e-03
 AAR converged to a relative residual of 8.94807e-05 in 17 iterations.

Density got negative

 AAR converged to a relative residual of 2.65696e-07 in 37 iterations.
 Poisson problem took 0.442826s
 This SCF iteration took 1.893 s.

 ========================
 Relaxation iteration:  7
 SCF iteration number:  2
 ========================
 Fermi energy = -0.034312
 ------------------
 Eband = -12.98072066
 Exc = -10.71248691
 Exc_dc = -12.08915768
 Eelec_dc = 23.39933662
 Eent = -0.00000007
 E_corr = 0.00145896
 Eself = 69.85032208
 Etot = -58.05357645
 ------------------
 Etot = -58.05357645
 Eatom = -29.02678823
 Error in SCF iteration: 3.8871e-03
 AAR converged to a relative residual of 2.41478e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 1.16089e-07 in 43 iterations.
 Poisson problem took 0.493299s
 This SCF iteration took 1.836 s.

 ========================
 Relaxation iteration:  7
 SCF iteration number:  3
 ========================
 Fermi energy = -0.034931
 ------------------
 Eband = -13.01331906
 Exc = -10.70783274
 Exc_dc = -12.08269214
 Eelec_dc = 23.43340982
 Eent = -0.00000007
 E_corr = 0.00145896
 Eself = 69.85032208
 Etot = -58.05391302
 ------------------
 Etot = -58.05391302
 Eatom = -29.02695651
 Error in SCF iteration: 8.8490e-04
 AAR converged to a relative residual of 2.10455e-05 in 19 iterations.

Density got negative
```

```
 AAR converged to a relative residual of 1.46274e-07 in 37 iterations.
 Poisson problem took 0.422173s
 This SCF iteration took 1.809 s.

 ========================
 Relaxation iteration:  7
 SCF iteration number:  4
 ========================
 Fermi energy = -0.034736
 ------------------
 Eband = -13.01803664
 Exc = -10.70734981
 Exc_dc = -12.08197174
 Eelec_dc = 23.43834356
 Eent = -0.00000007
 E_corr = 0.00145896
 Eself = 69.85032208
 Etot = -58.05393434
 ------------------
 Etot = -58.05393434
 Eatom = -29.02696717
 Error in SCF iteration: 5.3927e-04
 AAR converged to a relative residual of 5.17347e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 1.89802e-07 in 37 iterations.
 Poisson problem took 0.416471s
 This SCF iteration took 1.746 s.

 ========================
 Relaxation iteration:  7
 SCF iteration number:  5
 ========================
 Fermi energy = -0.035030
 ------------------
 Eband = -13.02056237
 Exc = -10.70738476
 Exc_dc = -12.08191958
 Eelec_dc = 23.44094705
 Eent = -0.00000007
 E_corr = 0.00145896
 Eself = 69.85032208
 Etot = -58.05394369
 ------------------
 Etot = -58.05394369
 Eatom = -29.02697184
 Error in SCF iteration: 9.9563e-05
 AAR converged to a relative residual of 4.59387e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 2.11901e-07 in 31 iterations.
 Poisson problem took 0.376474s
 This SCF iteration took 1.742 s.

 ========================
 Relaxation iteration:  7
 SCF iteration number:  6
 ========================
 Fermi energy = -0.035095
 ------------------
 Eband = -13.02179417
```

```
 Exc = -10.70724079
 Exc_dc = -12.08173065
 Eelec_dc = 23.44222287
 Eent = -0.00000007
 E_corr = 0.00145896
 Eself = 69.85032208
 Etot = -58.05394461
 ------------------
 Etot = -58.05394461
 Eatom = -29.02697231
 Error in SCF iteration: 7.0329e-05
 AAR converged to a relative residual of 7.85684e-05 in 20 iterations.

Density got negative

 AAR converged to a relative residual of 7.94725e-08 in 37 iterations.
 Poisson problem took 0.417464s
 This SCF iteration took 1.758 s.

 ========================
 Relaxation iteration:  7
 SCF iteration number:  7
 ========================
 Fermi energy = -0.035233
 ------------------
 Eband = -13.02355349
 Exc = -10.70708143
 Exc_dc = -12.08151761
 Eelec_dc = 23.44403556
 Eent = -0.00000007
 E_corr = 0.00145896
 Eself = 69.85032208
 Etot = -58.05394493
 ------------------
 Etot = -58.05394493
 Eatom = -29.02697247
 Error in SCF iteration: 3.2972e-05
 AAR converged to a relative residual of 6.17223e-05 in 19 iterations.

Density got negative

 AAR converged to a relative residual of 2.40326e-07 in 31 iterations.
 Poisson problem took 0.363022s
 This SCF iteration took 1.736 s.

 ========================
 Relaxation iteration:  7
 SCF iteration number:  8
 ========================
 Fermi energy = -0.035327
 ------------------
 Eband = -13.02398322
 Exc = -10.70705775
 Exc_dc = -12.08148454
 Eelec_dc = 23.44447343
 Eent = -0.00000007
 E_corr = 0.00145896
 Eself = 69.85032208
 Etot = -58.05394619
 ------------------
 Etot = -58.05394619
 Eatom = -29.02697309
 Error in SCF iteration: 1.4191e-05
 AAR converged to a relative residual of 6.12757e-05 in 19 iterations.
```

```
Density got negative

 AAR converged to a relative residual of 2.70192e-07 in 20 iterations.
 Poisson problem took 0.275905s
 This SCF iteration took 1.626 s.


 Finished SCF iteration in 8 steps!
 ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~

 ***********************************************************
 *          Energy per unit cell = -58.053946190 Ha.       *
 *          Energy per atom = -29.026973095 Ha.            *
 ***********************************************************

 Starting atomic force calculation ...
 WARNING: Atom 2 too close to boundary for b calculation
 local force calculation: 0.085 s
 ***********************************************************
 *                      Atomic Force                       *
 ***********************************************************
 Drift free forces (Ha/Bohr):
  -0.340537552447706   0.000000036796219   0.000000058852151
   0.340537552447706  -0.000000036796219  -0.000000058852151

 Max magnitude of forces (Ha/Bohr):   0.340537552447713


 Time for calculating forces: 0.173500 s.

 Relaxation step number 7 completed in 15.247283 s.
 ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~

 ######################################################################
 Relaxation step number: 8

 Starting pseudocharge generation and self energy calculation...
 WARNING: Atom 1 too close to boundary for b calculation
 WARNING: Atom 2 too close to boundary for b calculation
 Integration b = 16.000001857891

 Integration b_ref = 15.999999999995

 ***************************************
 *          Eself_ref = 231.832536       *
 ***************************************
 Done. (0.037215 s)
 Time for b calculation: 0.051 seconds.

 Starting calculating nonlocal projectors ...
 Done. (0.006383 s)

 ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
 Starting SCF iteration...
 AAR converged to a relative residual of 2.96476e-07 in 76 iterations.
 Poisson problem took 0.827868s
 ============================================
 Relaxation iteration:  8
 SCF iteration number:  1, Chebyshev cycle: 1
 ============================================
 Fermi energy = -0.030311
 ------------------
 Eband = -12.82399943
```

```
Exc = -10.68350234
Exc...
```

```
rmpath(MSPARC_root);
rmpath(fullfile(MSPARC_root,"src"));
rmpath("M-SPARC\");
```

Next we run geometry optimization in KSSOLV. We need to use function "relaxatoms" for this purpose.

```
% path and check
addpath(KSSOLV_root);
addpath("KSSOLV\");
KSSOLV_startup;
[K_mol3,K_Ham3,K_wf3,K_info3] = kssolv_geoopt(atom1,atom2,L2,d,Ecut2);
```

```
The pseudopotential for Na is loaded from C:\Users\tvekua\OneDrive - MathWorks\Desktop\DFTMaterial\KSSOLV\/ppdata/de
The pseudopotential for Cl is loaded from C:\Users\tvekua\OneDrive - MathWorks\Desktop\DFTMaterial\KSSOLV\/ppdata/de
The pseudopotential for Na is loaded from C:\Users\tvekua\OneDrive - MathWorks\Desktop\DFTMaterial\KSSOLV\/ppdata/de
The pseudopotential for Cl is loaded from C:\Users\tvekua\OneDrive - MathWorks\Desktop\DFTMaterial\KSSOLV\/ppdata/de
Regular SCF for Pure DFT
Beging SCF calculation for □Í...
SCF iter   1:
eigtol =   1.000e-02
Rel Vtot Err    =            2.706e-01
Total Energy    = -4.6077794281887e+01
SCF iter   2:
eigtol =   1.000e-02
Rel Vtot Err    =            3.834e-02
Total Energy    = -4.7138689462095e+01
SCF iter   3:
eigtol =   4.793e-03
Rel Vtot Err    =            2.777e-02
Total Energy    = -4.7215731303151e+01
SCF iter   4:
eigtol =   3.471e-03
Rel Vtot Err    =            1.554e-03
Total Energy    = -4.7238307597986e+01
SCF iter   5:
eigtol =   1.942e-04
Rel Vtot Err    =            2.253e-04
Total Energy    = -4.7238320142749e+01
SCF iter   6:
eigtol =   2.816e-05
Rel Vtot Err    =            1.037e-05
Total Energy    = -4.7238320233109e+01
SCF iter   7:
eigtol =   1.296e-06
Rel Vtot Err    =            1.032e-06
Total Energy    = -4.7238320234276e+01
SCF iter   8:
eigtol =   1.290e-07
Rel Vtot Err    =            6.664e-08
Total Energy    = -4.7238320234284e+01
SCF iter   9:
eigtol =   8.329e-09
Rel Vtot Err    =            1.133e-08
Total Energy    = -4.7238320234284e+01
SCF iter  10:
eigtol =   1.417e-09
Rel Vtot Err    =            3.739e-09
Total Energy    = -4.7238320234284e+01
```

```
Convergence is reached!
resnrm =   1.370e-08
resnrm =   1.052e-08
resnrm =   4.777e-07
resnrm =   4.778e-07
---------------------
Elapsed time is 6.584524 seconds.
Etot            = -4.7238320234284e+01
Eone-electron   = -6.6494500616407e+01
Ehartree        =  2.3682086399281e+01
Exc             = -6.0614460905249e+00
Eewald          =  1.6355400733659e+00
Ealphat         =  0.0000000000000e+00
-------------------------------------
Total time used =            9.703e+00
||HX-XD||_F     =            6.758e-07
starting bond length =   2.000e+00 (Bohr)
Starting SCF4M calculation for □Í...
eigtol =   1.000e-02
Rel Vtot Err    =            6.278e-01
Total Energy    = -4.4285540176657e+01
eigtol =   1.000e-02
Rel Vtot Err    =            2.130e-01
Total Energy    = -4.7153543882986e+01
eigtol =   1.000e-02
Rel Vtot Err    =            3.652e-02
Total Energy    = -4.7173288016348e+01
eigtol =   4.565e-03
Rel Vtot Err    =            1.340e-02
Total Energy    = -4.7232387940388e+01
eigtol =   1.675e-03
Rel Vtot Err    =            2.129e-03
Total Energy    = -4.7238166531788e+01
eigtol =   2.662e-04
Rel Vtot Err    =            3.331e-04
Total Energy    = -4.7238314578445e+01
eigtol =   4.164e-05
Rel Vtot Err    =            1.007e-04
Total Energy    = -4.7238315450512e+01
eigtol =   1.259e-05
Rel Vtot Err    =            2.825e-05
Total Energy    = -4.7238315466369e+01
eigtol =   3.532e-06
Rel Vtot Err    =            6.826e-06
Total Energy    = -4.7238315467788e+01
SCF iter  10:
eigtol =   8.532e-07
Rel Vtot Err    =            1.995e-06
Total Energy    = -4.7238315467904e+01
Etot            = -4.7238315467904e+01
Entropy         =  0.0000000000000e+00
Ekin            = -2.7006698673054e+01
Eewald          =  1.6355400733659e+00
Ealphat         =  0.0000000000000e+00
Ecor            = -3.9487772590328e+01
Ecoul           =  2.3682048559504e+01
Exc             = -6.0614328373925e+00
-------------------------------------
Total time used =            3.078e+00
||HX-XD||_F     =            4.794e-06
fval = -4.723831546790367e+01
norm(g) =   1.532e+01
```

```
   Diagnostic Information

Number of variables: 6

Functions
Objective and gradient:              @(x)ksfg(x,mol,ksopts)
Hessian:                             bfgs


Algorithm selected
   quasi-newton


_____________________________________________________________
   End diagnostic information
Starting SCF4M calculation for □Í...
eigtol =   1.000e-02
Rel Vtot Err    =            3.069e-01
Total Energy    =  9.4936104052313e+00
eigtol =   1.000e-02
Rel Vtot Err    =            3.789e-02
Total Energy    =  6.3142390261875e+00
eigtol =   4.736e-03
Rel Vtot Err    =            1.257e-02
Total Energy    =  6.2189828785661e+00
eigtol =   1.572e-03
Rel Vtot Err    =            1.034e-03
Total Energy    =  6.2159225622148e+00
eigtol =   1.293e-04
Rel Vtot Err    =            1.896e-04
Total Energy    =  6.2158857726552e+00
eigtol =   2.370e-05
Rel Vtot Err    =            4.430e-05
Total Energy    =  6.2158855847997e+00
eigtol =   5.538e-06
Rel Vtot Err    =            4.341e-06
Total Energy    =  6.2158855811479e+00
eigtol =   5.426e-07
Rel Vtot Err    =            7.464e-07
Total Energy    =  6.2158855806815e+00
eigtol =   9.331e-08
Rel Vtot Err    =            2.082e-07
Total Energy    =  6.2158855806754e+00
SCF iter  10:
eigtol =   2.602e-08
Rel Vtot Err    =            4.759e-08
Total Energy    =  6.2158855806750e+00
Etot            =  6.2158855806750e+00
Entropy         =  0.0000000000000e+00
Ekin            = -4.2017401465442e+01
Eewald          =  7.2834740346657e+01
Ealphat         =  0.0000000000000e+00
Ecor            = -4.4618685350560e+01
Ecoul           =  2.6572698893358e+01
Exc             = -6.5554668433377e+00
-------------------------------------
Total time used =            3.656e+00
||HX-XD||_F     =            3.507e-07
fval =  6.215885580675025e+00
norm(g) =   9.904e-05
Starting SCF4M calculation for □Í...
eigtol =   1.000e-02
Rel Vtot Err    =            3.736e-01
Total Energy    = -4.3547587291535e+01
```

```
eigtol =   1.000e-02
Rel Vtot Err    =            4.367e-02
Total Energy    = -4.6419187883067e+01
eigtol =   5.459e-03
Rel Vtot Err    =            1.221e-02
Total Energy    = -4.6479798906036e+01
eigtol =   1.526e-03
Rel Vtot Err    =            3.581e-03
Total Energy    = -4.6483315599673e+01
eigtol =   4.477e-04
Rel Vtot Err    =            4.297e-04
Total Energy    = -4.6483789983864e+01
eigtol =   5.371e-05
Rel Vtot Err    =            1.091e-04
Total Energy    = -4.6483791642136e+01
eigtol =   1.364e-05
Rel Vtot Err    =            1.773e-05
Total Energy    = -4.6483791650383e+01
eigtol =   2.217e-06
Rel Vtot Err    =            4.954e-06
Total Energy    = -4.6483791654478e+01
eigtol =   6.192e-07
Rel Vtot Err    =            1.221e-06
Total Energy    = -4.6483791654628e+01
SCF iter  10:
eigtol =   1.526e-07
Rel Vtot Err    =            2.676e-07
Total Energy    = -4.6483791654632e+01
Etot            = -4.6483791654632e+01
Entropy         =  0.0000000000000e+00
Ekin            = -2.8814114508617e+01
Eewald          =  5.0672960165567e+00
Ealphat         =  0.0000000000000e+00
Ecor            = -4.1106184323647e+01
Ecoul           =  2.4605215287114e+01
Exc             = -6.2360041260376e+00
---------------------------------------
Total time used =            3.234e+00
||HX-XD||_F     =            7.949e-07
fval = -4.648379165463157e+01
norm(g) =   1.702e+01
Starting SCF4M calculation for □Í...
eigtol =   1.000e-02
Rel Vtot Err    =            4.762e-02
Total Energy    = -4.6736033434925e+01
eigtol =   5.952e-03
Rel Vtot Err    =            2.073e-02
Total Energy    = -4.7152438873722e+01
eigtol =   2.591e-03
Rel Vtot Err    =            8.520e-03
Total Energy    = -4.7155114003158e+01
eigtol =   1.065e-03
Rel Vtot Err    =            1.962e-03
Total Energy    = -4.7155131469297e+01
eigtol =   2.452e-04
Rel Vtot Err    =            3.986e-04
Total Energy    = -4.7155200175476e+01
eigtol =   4.982e-05
Rel Vtot Err    =            1.070e-04
Total Energy    = -4.7155201442096e+01
eigtol =   1.337e-05
Rel Vtot Err    =            1.158e-05
Total Energy    = -4.7155201468199e+01
eigtol =   1.447e-06
```

```
Rel Vtot Err    =            4.270e-06
Total Energy    = -4.7155201469745e+01
eigtol =   5.337e-07
Rel Vtot Err    =            9.750e-07
Total Energy    = -4.7155201469948e+01
SCF iter  10:
eigtol =   1.219e-07
Rel Vtot Err    =            2.195e-07
Total Energy    = -4.7155201469954e+01
Etot            = -4.7155201469954e+01
Entropy         =  0.0000000000000e+00
Ekin            = -2.7244272496375e+01
Eewald          =  2.0740905521993e+00
Ealphat         =  0.0000000000000e+00
Ecor            = -3.9707505393625e+01
Ecoul           =  2.3807012771163e+01
Exc             = -6.0845269033174e+00
---------------------------------------
Total time used =            3.000e+00
||HX-XD||_F     =            6.364e-07
fval = -4.715520146995448e+01
norm(g) =   1.560e+01
Starting SCF4M calculation for □Í...
eigtol =   1.000e-02
Rel Vtot Err    =            7.376e-02
Total Energy    = -4.6099186170103e+01
eigtol =   9.220e-03
Rel Vtot Err    =            8.312e-02
Total Energy    = -4.7056526037860e+01
eigtol =   9.220e-03
Rel Vtot Err    =            3.885e-02
Total Energy    = -4.7194709811522e+01
eigtol =   4.857e-03
Rel Vtot Err    =            2.451e-02
Total Energy    = -4.7213240726144e+01
eigtol =   3.063e-03
Rel Vtot Err    =            1.992e-02
Total Energy    = -4.7217747487415e+01
eigtol =   2.490e-03
Rel Vtot Err    =            1.761e-02
Total Energy    = -4.7218471250151e+01
eigtol =   2.201e-03
Rel Vtot Err    =            1.498e-02
Total Energy    = -4.7221024813954e+01
eigtol =   1.872e-03
Rel Vtot Err    =            7.699e-03
Total Energy    = -4.7224671763771e+01
eigtol =   9.623e-04
Rel Vtot Err    =            4.673e-03
Total Energy    = -4.7225421731163e+01
SCF iter  10:
eigtol =   5.842e-04
Rel Vtot Err    =            2.694e-03
Total Energy    = -4.7225747891140e+01
Etot            = -4.7225747891140e+01
Entropy         =  0.0000000000000e+00
Ekin            = -2.7117955576159e+01
Eewald          =  1.7022777270358e+00
Ealphat         =  0.0000000000000e+00
Ecor            = -3.9486109963975e+01
Ecoul           =  2.3750056303497e+01
Exc             = -6.0740163815392e+00
---------------------------------------
Total time used =            2.719e+00
```

```
||HX-XD||_F     =            4.676e-03
fval = -4.722574789114048e+01
norm(g) =   1.536e+01
Starting SCF4M calculation for □Í...
eigtol =   1.000e-02
Rel Vtot Err    =            1.428e-01
Total Energy    = -4.5116295583060e+01
eigtol =   1.000e-02
Rel Vtot Err    =            1.483e-01
Total Energy    = -4.6797647191135e+01
eigtol =   1.000e-02
Rel Vtot Err    =            7.390e-02
Total Energy    = -4.7137270864119e+01
eigtol =   9.237e-03
Rel Vtot Err    =            4.985e-02
Total Energy    = -4.7188172922300e+01
eigtol =   6.231e-03
Rel Vtot Err    =            4.006e-02
Total Energy    = -4.7201957488463e+01
eigtol =   5.008e-03
Rel Vtot Err    =            3.636e-02
Total Energy    = -4.7207684626978e+01
eigtol =   4.545e-03
Rel Vtot Err    =            3.154e-02
Total Energy    = -4.7214747973058e+01
eigtol =   3.943e-03
Rel Vtot Err    =            2.449e-02
Total Energy    = -4.7224550650483e+01
eigtol =   3.061e-03
Rel Vtot Err    =            2.426e-02
Total Energy    = -4.7224400524084e+01
SCF iter  10:
eigtol =   3.033e-03
Rel Vtot Err    =            2.379e-02
Total Energy    = -4.7224539507462e+01
Etot            = -4.7224539507462e+01
Entropy         =  0.0000000000000e+00
Ekin            = -2.7740143163005e+01
Eewald          =  1.6458986769761e+00
Ealphat         =  0.0000000000000e+00
Ecor            = -3.9122331560589e+01
Ecoul           =  2.4138516050252e+01
Exc             = -6.1464795110967e+00
---------------------------------------
Total time used =            2.516e+00
||HX-XD||_F     =            9.660e-03
fval = -4.722453950746242e+01
norm(g) =   1.529e+01
Starting SCF4M calculation for □Í...
eigtol =   1.000e-02
Rel Vtot Err    =            3.344e-02
Total Energy    = -4.6928656885561e+01
eigtol =   4.181e-03
Rel Vtot Err    =            3.127e-02
Total Energy    = -4.7204783017772e+01
eigtol =   3.909e-03
Rel Vtot Err    =            1.150e-02
Total Energy    = -4.7236184618070e+01
eigtol =   1.438e-03
Rel Vtot Err    =            9.718e-03
Total Energy    = -4.7236634685938e+01
eigtol =   1.215e-03
Rel Vtot Err    =            9.034e-03
Total Energy    = -4.7236683207951e+01
```

```
eigtol =   1.129e-03
Rel Vtot Err    =            7.782e-03
Total Energy    = -4.7237264410032e+01
eigtol =   9.728e-04
Rel Vtot Err    =            2.821e-03
Total Energy    = -4.7238003699090e+01
eigtol =   3.526e-04
Rel Vtot Err    =            8.902e-04
Total Energy    = -4.7238121587423e+01
eigtol =   1.113e-04
Rel Vtot Err    =            6.893e-04
Total Energy    = -4.7238122857257e+01
SCF iter  10:
eigtol =   8.617e-05
Rel Vtot Err    =            4.879e-04
Total Energy    = -4.7238122753223e+01
Etot            = -4.7238122753223e+01
Entropy         =  0.0000000000000e+00
Ekin            = -2.7006501953170e+01
Eewald          =  1.6365756116076e+00
Ealphat         =  0.0000000000000e+00
Ecor            = -3.9488065138987e+01
Ecoul           =  2.3681109087389e+01
Exc             = -6.0612403600626e+00
--------------------------------------
Total time used =            3.047e+00
||HX-XD||_F     =            4.934e-04
fval = -4.723812275322327e+01
norm(g) =   1.533e+01
Starting SCF4M calculation for □Í...
eigtol =   1.000e-02
Rel Vtot Err    =            8.353e-02
Total Energy    = -4.5726969333948e+01
eigtol =   1.000e-02
Rel Vtot Err    =            9.198e-02
Total Energy    = -4.7034171117505e+01
eigtol =   1.000e-02
Rel Vtot Err    =            4.294e-02
Total Energy    = -4.7199669305014e+01
eigtol =   5.368e-03
Rel Vtot Err    =            2.802e-02
Total Energy    = -4.7221772765162e+01
eigtol =   3.503e-03
Rel Vtot Err    =            2.317e-02
Total Energy    = -4.7227232051961e+01
eigtol =   2.896e-03
Rel Vtot Err    =            2.115e-02
Total Energy    = -4.7227944407350e+01
eigtol =   2.643e-03
Rel Vtot Err    =            2.028e-02
Total Energy    = -4.7228423380610e+01
eigtol =   2.535e-03
Rel Vtot Err    =            1.757e-02
Total Energy    = -4.7231853269839e+01
eigtol =   2.196e-03
Rel Vtot Err    =            1.776e-02
Total Energy    = -4.7231627725537e+01
SCF iter  10:
eigtol =   2.196e-03
Rel Vtot Err    =            1.575e-02
Total Energy    = -4.7232153286046e+01
Etot            = -4.7232153286046e+01
Entropy         =  0.0000000000000e+00
Ekin            = -2.7466173403517e+01
```

```
Eewald          =  1.6357017823804e+00
Ealphat         =  0.0000000000000e+00
Ecor            = -3.9284287753000e+01
Ecoul           =  2.4003896321202e+01
Exc             = -6.1212902331114e+00
---------------------------------------
Total time used =            2.875e+00
||HX-XD||_F     =            1.523e-02
fval = -4.723215328604585e+01
norm(g) =   1.527e+01
Starting SCF4M calculation for □Í...
eigtol =   1.000e-02
Rel Vtot Err    =            3.846e-02
Total Energy    = -4.6736219864979e+01
eigtol =   4.807e-03
Rel Vtot Err    =            3.932e-02
Total Energy    = -4.7186898466151e+01
eigtol =   4.807e-03
Rel Vtot Err    =            1.535e-02
Total Energy    = -4.7233982488393e+01
eigtol =   1.919e-03
Rel Vtot Err    =            1.191e-02
Total Energy    = -4.7235496178584e+01
eigtol =   1.489e-03
Rel Vtot Err    =            1.103e-02
Total Energy    = -4.7235598182366e+01
eigtol =   1.379e-03
Rel Vtot Err    =            1.005e-02
Total Energy    = -4.7236438717387e+01
eigtol =   1.256e-03
Rel Vtot Err    =            8.847e-03
Total Energy    = -4.7236548980910e+01
eigtol =   1.106e-03
Rel Vtot Err    =            7.666e-03
Total Energy    = -4.7237189601003e+01
eigtol =   9.583e-04
Rel Vtot Err    =            2.921e-03
Total Energy    = -4.7238163929293e+01
SCF iter  10:
eigtol =   3.652e-04
Rel Vtot Err    =            1.695e-03
Total Energy    = -4.7238262521420e+01
Etot            = -4.7238262521420e+01
Entropy         =  0.0000000000000e+00
Ekin            = -2.7031414999740e+01
Eewald          =  1.6355562441905e+00
Ealphat         =  0.0000000000000e+00
Ecor            = -3.9484145389533e+01
Ecoul           =  2.3707967743434e+01
Exc             = -6.0662261197712e+00
---------------------------------------
Total time used =            2.844e+00
||HX-XD||_F     =            3.714e-03
fval = -4.723826252142027e+01
norm(g) =   1.530e+01
Starting SCF4M calculation for □Í...
eigtol =   1.000e-02
Rel Vtot Err    =            1.397e-01
Total Energy    = -4.5222949290623e+01
eigtol =   1.000e-02
Rel Vtot Err    =            1.464e-01
Total Energy    = -4.6805776727422e+01
eigtol =   1.000e-02
Rel Vtot Err    =            7.259e-02
```

```
Total Energy    = -4.7140739299973e+01
eigtol =   9.074e-03
Rel Vtot Err    =            4.788e-02
Total Energy    = -4.7192968747758e+01
eigtol =   5.986e-03
Rel Vtot Err    =            3.977e-02
Total Energy    = -4.7203842405550e+01
eigtol =   4.971e-03
Rel Vtot Err    =            3.627e-02
Total Energy    = -4.7209663531164e+01
eigtol =   4.534e-03
Rel Vtot Err    =            3.128e-02
Total Energy    = -4.7216717121051e+01
eigtol =   3.911e-03
Rel Vtot Err    =            2.402e-02
Total Energy    = -4.7226691459513e+01
eigtol =   3.003e-03
Rel Vtot Err    =            2.372e-02
Total Energy    = -4.7226574134695e+01
SCF iter  10:
eigtol =   2.965e-03
Rel Vtot Err    =            2.326e-02
Total Energy    = -4.7226730794225e+01
Etot            = -4.7226730794225e+01
Entropy         =  0.0000000000000e+00
Ekin            = -2.7716705380130e+01
Eewald          =  1.6355416904485e+00
Ealphat         =  0.0000000000000e+00
Ecor            = -3.9130457671748e+01
Ecoul           =  2.4129693231195e+01
Exc             = -6.1448026639908e+00
---------------------------------------
Total time used =            3.328e+00
||HX-XD||_F     =            9.663e-03
fval = -4.722673079422540e+01
norm(g) =   1.528e+01
Starting SCF4M calculation for □Í...
eigtol =   1.000e-02
Rel Vtot Err    =            3.262e-02
Total Energy    = -4.6987203311404e+01
eigtol =   4.078e-03
Rel Vtot Err    =            3.060e-02
Total Energy    = -4.7206644123208e+01
eigtol =   3.825e-03
Rel Vtot Err    =            1.089e-02
Total Energy    = -4.7236434339353e+01
eigtol =   1.362e-03
Rel Vtot Err    =            9.253e-03
Total Energy    = -4.7236886877302e+01
eigtol =   1.157e-03
Rel Vtot Err    =            8.714e-03
Total Energy    = -4.7236924026824e+01
eigtol =   1.089e-03
Rel Vtot Err    =            7.675e-03
Total Energy    = -4.7237421399132e+01
eigtol =   9.594e-04
Rel Vtot Err    =            3.632e-03
Total Energy    = -4.7238100265272e+01
eigtol =   4.540e-04
Rel Vtot Err    =            7.766e-04
Total Energy    = -4.7238312507079e+01
eigtol =   9.707e-05
Rel Vtot Err    =            6.232e-04
Total Energy    = -4.7238315307458e+01
```

```
SCF iter  10:
eigtol =   7.789e-05
Rel Vtot Err    =            5.340e-04
Total Energy    = -4.7238313493362e+01
Etot            = -4.7238313493362e+01
Entropy         =  0.0000000000000e+00
Ekin            = -2.7003601752763e+01
Eewald          =  1.6355402350744e+00
Ealphat         =  0.0000000000000e+00
Ecor            = -3.9487640850283e+01
Ecoul           =  2.3678064592087e+01
Exc             = -6.0606757174780e+00
---------------------------------------
Total time used =            3.172e+00
||HX-XD||_F     =            5.986e-04
fval = -4.723831349336204e+01
norm(g) =   1.533e+01
Starting SCF4M calculation for □Í...
eigtol =   1.000e-02
Rel Vtot Err    =            4.960e-02
Total Energy    = -4.6327206085114e+01
eigtol =   6.200e-03
Rel Vtot Err    =            5.671e-02
Total Energy    = -4.7144087437231e+01
eigtol =   6.200e-03
Rel Vtot Err    =            2.513e-02
Total Energy    = -4.7225533878025e+01
eigtol =   3.141e-03
Rel Vtot Err    =            1.707e-02
Total Energy    = -4.7231894554918e+01
eigtol =   2.134e-03
Rel Vtot Err    =            1.456e-02
Total Energy    = -4.7233359045814e+01
eigtol =   1.820e-03
Rel Vtot Err    =            1.342e-02
Total Energy    = -4.7234162878169e+01
eigtol =   1.677e-03
Rel Vtot Err    =            1.191e-02
Total Energy    = -4.7235088059552e+01
eigtol =   1.489e-03
Rel Vtot Err    =            9.722e-03
Total Energy    = -4.7236380236919e+01
eigtol =   1.215e-03
Rel Vtot Err    =            9.556e-03
Total Energy    = -4.7236378098439e+01
SCF iter  10:
eigtol =   1.194e-03
Rel Vtot Err    =            9.049e-03
Total Energy    = -4.7236457607437e+01
Etot            = -4.7236457607437e+01
Entropy         =  0.0000000000000e+00
Ekin            = -2.7203574439352e+01
Eewald          =  1.6355400895380e+00
Ealphat         =  0.0000000000000e+00
Ecor            = -3.9426410785672e+01
Ecoul           =  2.3850777741164e+01
Exc             = -6.0927902131158e+00
---------------------------------------
Total time used =            3.141e+00
||HX-XD||_F     =            3.725e-03
fval = -4.723645760743745e+01
norm(g) =   1.524e+01
Starting SCF4M calculation for □Í...
eigtol =   1.000e-02
```

```
Rel Vtot Err    =            3.081e-02
Total Energy    = -4.6869446194506e+01
eigtol =   3.851e-03
Rel Vtot Err    =            3.152e-02
Total Energy    = -4.7207795135643e+01
eigtol =   3.851e-03
Rel Vtot Err    =            1.309e-02
Total Energy    = -4.7236047370961e+01
eigtol =   1.636e-03
Rel Vtot Err    =            1.018e-02
Total Energy    = -4.7236516053528e+01
eigtol =   1.273e-03
Rel Vtot Err    =            9.261e-03
Total Energy    = -4.7236875964388e+01
eigtol =   1.158e-03
Rel Vtot Err    =            8.456e-03
Total Energy    = -4.7236974854608e+01
eigtol =   1.057e-03
Rel Vtot Err    =            8.339e-03
Total Energy    = -4.7237037580758e+01
eigtol =   1.042e-03
Rel Vtot Err    =            6.504e-03
Total Energy    = -4.7237711731124e+01
eigtol =   8.130e-04
Rel Vtot Err    =            5.735e-03
Total Energy    = -4.7237782263291e+01
SCF iter  10:
eigtol =   7.169e-04
Rel Vtot Err    =            4.917e-03
Total Energy    = -4.7237926970847e+01
Etot            = -4.7237926970847e+01
Entropy         =  0.0000000000000e+00
Ekin            = -2.7061491637644e+01
Eewald          =  1.6355400749838e+00
Ealphat         =  0.0000000000000e+00
Ecor            = -3.9489335410328e+01
Ecoul           =  2.3751673762754e+01
Exc             = -6.0743137606122e+00
---------------------------------------
Total time used =            2.719e+00
||HX-XD||_F     =            6.275e-03
fval = -4.723792697084681e+01
norm(g) =   1.526e+01
Starting SCF4M calculation for □Í...
eigtol =   1.000e-02
Rel Vtot Err    =            2.561e-02
Total Energy    = -4.6933942133204e+01
eigtol =   3.201e-03
Rel Vtot Err    =            2.586e-02
Total Energy    = -4.7219348056517e+01
eigtol =   3.201e-03
Rel Vtot Err    =            1.139e-02
Total Energy    = -4.7237044113718e+01
eigtol =   1.424e-03
Rel Vtot Err    =            8.738e-03
Total Energy    = -4.7237229832008e+01
eigtol =   1.092e-03
Rel Vtot Err    =            7.924e-03
Total Energy    = -4.7237307536326e+01
eigtol =   9.905e-04
Rel Vtot Err    =            7.371e-03
Total Energy    = -4.7237628330475e+01
eigtol =   9.214e-04
Rel Vtot Err    =            7.298e-03
```

```
Total Energy    = -4.7237631060968e+01
eigtol =   9.123e-04
Rel Vtot Err    =            6.874e-03
Total Energy    = -4.7237662950683e+01
eigtol =   8.592e-04
Rel Vtot Err    =            6.706e-03
Total Energy    = -4.7237677909596e+01
SCF iter  10:
eigtol =   8.382e-04
Rel Vtot Err    =            6.001e-03
Total Energy    = -4.7237772259054e+01
Etot            = -4.7237772259054e+01
Entropy         =  0.0000000000000e+00
Ekin            = -2.7070157559335e+01
Eewald          =  1.6355400735282e+00
Ealphat         =  0.0000000000000e+00
Ecor            = -3.9492099833891e+01
Ecoul           =  2.3765896563938e+01
Exc             = -6.0769515032936e+00
-------------------------------------
Total time used =            2.391e+00
||HX-XD||_F     =            4.688e-03
fval = -4.723777225905351e+01
norm(g) =   1.525e+01
Starting SCF4M calculation for □Í...
eigtol =   1.000e-02
Rel Vtot Err    =            4.030e-02
Total Energy    = -4.6498551636785e+01
eigtol =   5.037e-03
Rel Vtot Err    =            4.273e-02
Total Energy    = -4.7182500078703e+01
eigtol =   5.037e-03
Rel Vtot Err    =            1.855e-02
Total Energy    = -4.7233095972526e+01
eigtol =   2.319e-03
Rel Vtot Err    =            1.376e-02
Total Energy    = -4.7234530866249e+01
eigtol =   1.720e-03
Rel Vtot Err    =            1.194e-02
Total Energy    = -4.7235901527531e+01
eigtol =   1.492e-03
Rel Vtot Err    =            1.100e-02
Total Energy    = -4.7236029688870e+01
eigtol =   1.375e-03
Rel Vtot Err    =            1.012e-02
Total Energy    = -4.7236230124878e+01
eigtol =   1.266e-03
Rel Vtot Err    =            9.426e-03
Total Energy    = -4.7236391034772e+01
eigtol =   1.178e-03
Rel Vtot Err    =            7.625e-03
Total Energy    = -4.7237356711283e+01
SCF iter  10:
eigtol =   9.531e-04
Rel Vtot Err    =            7.485e-03
Total Energy    = -4.7237341784804e+01
Etot            = -4.7237341784804e+01
Entropy         =  0.0000000000000e+00
Ekin            = -2.7119126103911e+01
Eewald          =  1.6355400733820e+00
Ealphat         =  0.0000000000000e+00
Ecor            = -3.9471340938106e+01
Ecoul           =  2.3801063058403e+01
Exc             = -6.0834778745719e+00
```

```
---------------------------------------
Total time used =            2.281e+00
||HX-XD||_F     =            5.219e-03
fval = -4.723734178480356e+01
norm(g) =   1.524e+01
Starting SCF4M calculation for □Í...
eigtol =   1.000e-02
Rel Vtot Err    =            5.105e-02
Total Energy    = -4.6395076559469e+01
eigtol =   6.381e-03
Rel Vtot Err    =            5.769e-02
Total Energy    = -4.7130588237872e+01
eigtol =   6.381e-03
Rel Vtot Err    =            2.457e-02
Total Energy    = -4.7224228436214e+01
eigtol =   3.071e-03
Rel Vtot Err    =            1.693e-02
Total Energy    = -4.7231248099780e+01
eigtol =   2.117e-03
Rel Vtot Err    =            1.491e-02
Total Energy    = -4.7232531378575e+01
eigtol =   1.863e-03
Rel Vtot Err    =            1.415e-02
Total Energy    = -4.7232764109149e+01
eigtol =   1.769e-03
Rel Vtot Err    =            1.214e-02
Total Energy    = -4.7234804736885e+01
eigtol =   1.518e-03
Rel Vtot Err    =            1.212e-02
Total Energy    = -4.7234745023416e+01
eigtol =   1.515e-03
Rel Vtot Err    =            1.147e-02
Total Energy    = -4.7234852587135e+01
SCF iter  10:
eigtol =   1.434e-03
Rel Vtot Err    =            9.884e-03
Total Energy    = -4.7236030346565e+01
Etot            = -4.7236030346565e+01
Entropy         =  0.0000000000000e+00
Ekin            = -2.7215114681466e+01
Eewald          =  1.6355400733677e+00
Ealphat         =  0.0000000000000e+00
Ecor            = -3.9426735353455e+01
Ecoul           =  2.3865766947401e+01
Exc             = -6.0954873324126e+00
---------------------------------------
Total time used =            2.734e+00
||HX-XD||_F     =            5.671e-03
fval = -4.723603034656524e+01
norm(g) =   1.521e+01
Starting SCF4M calculation for □Í...
eigtol =   1.000e-02
Rel Vtot Err    =            2.868e-02
Total Energy    = -4.6917361373167e+01
eigtol =   3.584e-03
Rel Vtot Err    =            2.806e-02
Total Energy    = -4.7216103590817e+01
eigtol =   3.508e-03
Rel Vtot Err    =            1.178e-02
Total Energy    = -4.7236940591630e+01
eigtol =   1.472e-03
Rel Vtot Err    =            9.435e-03
Total Energy    = -4.7237141665769e+01
eigtol =   1.179e-03
```

```
Rel Vtot Err    =            8.782e-03
Total Energy    = -4.7237207872076e+01
eigtol =   1.098e-03
Rel Vtot Err    =            8.506e-03
Total Energy    = -4.7237257251520e+01
eigtol =   1.063e-03
Rel Vtot Err    =            7.703e-03
Total Energy    = -4.7237682660951e+01
eigtol =   9.628e-04
Rel Vtot Err    =            7.509e-03
Total Energy    = -4.7237666936279e+01
eigtol =   9.386e-04
Rel Vtot Err    =            7.262e-03
Total Energy    = -4.7237676824658e+01
SCF iter  10:
eigtol =   9.078e-04
Rel Vtot Err    =            6.355e-03
Total Energy    = -4.7237768592052e+01
Etot            = -4.7237768592052e+01
Entropy         =  0.0000000000000e+00
Ekin            = -2.7069993863413e+01
Eewald          =  1.6355400733661e+00
Ealphat         =  0.0000000000000e+00
Ecor            = -3.9491781760953e+01
Ecoul           =  2.3765327874501e+01
Exc             = -6.0768609155536e+00
--------------------------------------
Total time used =            2.328e+00
||HX-XD||_F     =            9.007e-03
fval = -4.723776859205162e+01
norm(g) =   1.524e+01
Starting SCF4M calculation for □Í...
eigtol =   1.000e-02
Rel Vtot Err    =            2.564e-02
Total Energy    = -4.6960239845961e+01
eigtol =   3.206e-03
Rel Vtot Err    =            2.641e-02
Total Energy    = -4.7217636539485e+01
eigtol =   3.206e-03
Rel Vtot Err    =            1.135e-02
Total Energy    = -4.7236841601306e+01
eigtol =   1.419e-03
Rel Vtot Err    =            8.697e-03
Total Energy    = -4.7237102942331e+01
eigtol =   1.087e-03
Rel Vtot Err    =            7.805e-03
Total Energy    = -4.7237371009130e+01
eigtol =   9.756e-04
Rel Vtot Err    =            6.998e-03
Total Energy    = -4.7237437662233e+01
eigtol =   8.747e-04
Rel Vtot Err    =            6.827e-03
Total Energy    = -4.7237487746671e+01
eigtol =   8.534e-04
Rel Vtot Err    =            5.580e-03
Total Energy    = -4.7237913721469e+01
eigtol =   6.975e-04
Rel Vtot Err    =            5.217e-03
Total Energy    = -4.7237911327353e+01
SCF iter  10:
eigtol =   6.522e-04
Rel Vtot Err    =            5.008e-03
Total Energy    = -4.7237925621808e+01
Etot            = -4.7237925621808e+01
```

```
Entropy         =  0.0000000000000e+00
Ekin            = -2.7058918043438e+01
Eewald          =  1.6355400733659e+00
Ealphat         =  0.0000000000000e+00
Ecor            = -3.9492562204305e+01
Ecoul           =  2.3752489573277e+01
Exc             = -6.0744750207082e+00
----------------------------------------
Total time used =            2.500e+00
||HX-XD||_F     =            3.270e-03
fval = -4.723792562180837e+01
norm(g) =   1.526e+01

Local minimum possible.

fminunc stopped because it cannot decrease the objective function
along the current search direction.

<stopping criteria details>
Starting SCF4M calculation for □Í...
eigtol =   1.000e-02
Rel Vtot Err    =            6.347e-01
Total Energy    = -4.4604968605158e+01
eigtol =   1.000e-02
Rel Vtot Err    =            6.059e-01
Total Energy    = -4.5008156467670e+01
eigtol =   1.000e-02
Rel Vtot Err    =            2.573e-01
Total Energy    = -4.3483666716318e+01
eigtol =   1.000e-02
Rel Vtot Err    =            2.803e-01
Total Energy    = -4.2900614126330e+01
eigtol =   1.000e-02
Rel Vtot Err    =            2.158e-01
Total Energy    = -4.4556267353211e+01
eigtol =   1.000e-02
Rel Vtot Err    =            7.366e-02
Total Energy    = -4.6918784060511e+01
eigtol =   9.208e-03
Rel Vtot Err    =            2.998e-02
Total Energy    = -4.7196446566178e+01
eigtol =   3.748e-03
Rel Vtot Err    =            1.329e-02
Total Energy    = -4.7234698685583e+01
eigtol =   1.661e-03
Rel Vtot Err    =            1.139e-02
Total Energy    = -4.7234066469928e+01
SCF iter  10:
eigtol =   1.424e-03
Rel Vtot Err    =            1.027e-02
Total Energy    = -4.7235761307757e+01
eigtol =   1.284e-03
Rel Vtot Err    =            1.067e-02
Total Energy    = -4.7236715798945e+01
eigtol =   1.284e-03
Rel Vtot Err    =            5.845e-03
Total Energy    = -4.7237840194309e+01
eigtol =   7.306e-04
Rel Vtot Err    =            9.168e-04
Total Energy    = -4.7238300982390e+01
eigtol =   1.146e-04
Rel Vtot Err    =            6.238e-04
Total Energy    = -4.7238308000369e+01
eigtol =   7.798e-05
```

```
Rel Vtot Err    =            4.612e-04
Total Energy    = -4.7238310587464e+01
eigtol =   5.766e-05
Rel Vtot Err    =            1.493e-04
Total Energy    = -4.7238314786207e+01
eigtol =   1.867e-05
Rel Vtot Err    =            6.749e-05
Total Energy    = -4.7238315446067e+01
eigtol =   8.436e-06
Rel Vtot Err    =            6.481e-05
Total Energy    = -4.7238315449201e+01
eigtol =   8.102e-06
Rel Vtot Err    =            4.079e-05
Total Energy    = -4.7238315460698e+01
SCF iter  20:
eigtol =   5.099e-06
Rel Vtot Err    =            1.596e-05
Total Energy    = -4.7238315466876e+01
eigtol =   1.996e-06
Rel Vtot Err    =            1.349e-05
Total Energy    = -4.7238315467101e+01
eigtol =   1.686e-06
Rel Vtot Err    =            1.044e-05
Total Energy    = -4.7238315467593e+01
eigtol =   1.305e-06
Rel Vtot Err    =            6.041e-06
Total Energy    = -4.7238315467699e+01
eigtol =   7.551e-07
Rel Vtot Err    =            2.632e-06
Total Energy    = -4.7238315467866e+01
eigtol =   3.290e-07
Rel Vtot Err    =            1.974e-06
Total Energy    = -4.7238315467879e+01
eigtol =   2.468e-07
Rel Vtot Err    =            1.271e-06
Total Energy    = -4.7238315467869e+01
eigtol =   1.588e-07
Rel Vtot Err    =            7.837e-07
Total Energy    = -4.7238315467912e+01
Convergence is reached!
Etot            = -4.7238315467912e+01
Entropy         =  0.0000000000000e+00
Ekin            = -2.7006725354709e+01
Eewald          =  1.6355400733659e+00
Ealphat         =  0.0000000000000e+00
Ecor            = -3.9487766542030e+01
Ecoul           =  2.3682073912516e+01
Exc             = -6.0614375570548e+00
-------------------------------------
Total time used =            8.031e+00
||HX-XD||_F     =            1.804e-06
optimized bond length =   2.000e+00 (Bohr)
```

```
rmpath(KSSOLV_root);
rmpath("KSSOLV\");
```

```
fprintf("The bond leght from M-SPARC is %.3f Bohr\n", norm(S3.atom_pos_t(1,:)-
S3.atom_pos_t(2,:)));
```

```
The bond leght from M-SPARC is 4.365 Bohr
```

```
fprintf("The bond leght from KSSOLV is %.3f Bohr\n", norm(K_mol3.xyzlist(1,:)-
K_mol3.xyzlist(2,:)));
```

```
The bond leght from KSSOLV is 2.000 Bohr
```

Crystals

Here, we present the calculation of crystal systems in M-SPARC and KSSOLV. We use FCC silicon as an example. To define a crystal, we need to define the **Bravais lattice** $\mathbf{R} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$. Here scale of lattice vectors is vector $[n_1, n_2, n_3]$. Matrix of lattice vectors is $[\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3]^T$.

```
Lat_scale4 =  [10.25 10.25 10.25];
Latvec4 =  [0.0 0.5 0.5; 0.5 0.0 0.5; 0.5 0.5 0.0];
```

Next, we define the atom symbols, numbe of atoms and their reduced coordinates.

```
atom_list4 = ["Si"];
natom_list4 =  [2];
coord4 =  [0 0 0; 0.25 0.25 0.25];
```

We introduce the **Bloch's theorem**. In realistic systems there are $\approx 10^{20}$ atoms in cubic millimetre - unformidable to treat by any numerical method. To describe the bulk properties of materials, we will use periodic boundary conditions. Although the edge of real macroscopic crystal spoils the periodicity, the atoms deep inside bulk can hardly be influenced by atoms at the edge. The **Bloch's theorem** says that for a periodic potential $V(\mathbf{r}+\mathbf{L}) = V(\mathbf{r})$ the eigenfunctions can be written in the form

$$\psi_j(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}u_{j\mathbf{k}}(\mathbf{r}), \qquad u_{j\mathbf{k}}(\mathbf{r}+\mathbf{L}) = u_{j\mathbf{k}}(\mathbf{r}).$$

Then we can define the **First Brillouin zone**: part of space closer to the origin than to any integer multiple of the reciprocal lattice vectors $\mathbf{k} = n_1\mathbf{b}_1 + n_2\mathbf{b}_2 + n_3\mathbf{b}_3$, where $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$ are reciprocal lattice vectors. Thus the summation over infinite number of unit cell becomes an integral over the first Brillouin zone:

$$\sum_{\mathbf{L}}^{\infty} \Rightarrow \int_{\mathbf{k}\in 1.\mathrm{BZ}} d\mathbf{k}$$

In practise the integral is replaced by a weighted sum of discrete K-points:

$$\int_{\mathbf{k}} d\mathbf{k} \approx \sum_{\mathbf{k}} w_{\mathbf{k}}$$

We need to do a convergence tests on the grids of discrete K-points in the first Brillouin zone for crystal simulation to get the physical results. Here we define the number of K-points along each direction for the sampling in First Brillouin zone n_k for both toolboxes.

```
nk4 = 2; % along each direction
```

Then we start the calculation in M-SPARC and select the mesh spacing again.

```
h4 = 0.5; % in Bohr

addpath(MSPARC_root);
addpath(fullfile(MSPARC_root,"src"));
addpath("M-SPARC\");
% Real space toolbox M-SPARC
msparc_crystal(Lat_scale4,Latvec4,atom_list4,natom_list4,coord4,h4,nk4,MSPARC_root);
S4 = msparc("M-SPARC/crystal");
```

```
 Reading .inpt file ...


<INPT>
# $ cat M-SPARC/crystal.inpt
LATVEC_SCALE: 10.250000 10.250000 10.250000
LATVEC: 0.000000 0.500000 0.500000
 0.500000 0.000000 0.500000
 0.500000 0.500000 0.000000
MESH_SPACING: 0.500000
KPOINT_GRID: 2 2 2
KPOINT_SHIFT: 0 0 0
BC: P P P
EXCHANGE_CORRELATION: GGA_PBE
SMEARING: 1E-8
<\INPT>

 Reading .ion file ...
 Number of atom types : 1
 Total number of atoms: 2
 Default atomic mass for Si is 28.085000
 pseudo_dir # 1 = 14_Si_4_1.9_1.9_pbe_n_v1.0.psp8

 COORD:
                   0                   0                   0
   1.811961126790528   1.811961126790528   1.811961126790528

atom type 1, l = 0, r_core read 1.91059, change to rmax where |UdV| < 1E-8, 1.93000.
atom type 1, l = 1, r_core read 1.91059, change to rmax where |UdV| < 1E-8, 1.93000.
atom type 1, l = 2, r_core read 1.91059, change to rmax where |UdV| < 1E-8, 1.93000.
 reduced kpoint grid before symmetry:
                   0                   0                   0
   0.500000000000000                   0                   0
                   0   0.500000000000000                   0
   0.500000000000000   0.500000000000000                   0
                   0                   0   0.500000000000000
   0.500000000000000                   0   0.500000000000000
                   0   0.500000000000000   0.500000000000000
   0.500000000000000   0.500000000000000   0.500000000000000

 reduced kpoint grid after symmetry:
                   0                   0                   0
   0.500000000000000                   0                   0
                   0   0.500000000000000                   0
   0.500000000000000   0.500000000000000                   0
                   0                   0   0.500000000000000
   0.500000000000000                   0   0.500000000000000
                   0   0.500000000000000   0.500000000000000
   0.500000000000000   0.500000000000000   0.500000000000000

 nspin = 1, nspinor = 1, nspden = 1
## Chebyshev polynomial degree not provided, finding npl ...
## Based on the mesh size, npl is set to: 18
```

```
## Number of states not provided, finding Nev ...
## Based on the number of electrons, Nev is set to: 10
## Based on the desired accuracy, SCF_tol is set to: 2.159e-04
## Poisson tolerance not provided, choosing poisson_tol ...
## poisson_tol is set to: 2.159e-06
## Pseudocharge tolerance not provided, choosing pseudocharge_tol ...
## pseudocharge_tol is set to: 2.159e-07
 Creating differentiation matrices ...
 Done. (0.311 sec)

 Estimated memory usage:
 Total:   21.78 MB
 orbitals            :   12.36 MB
 sparse matrices     :    8.70 MB
 global-size vectors :  369.14 kB
 mixing histories    :  369.14 kB

 Finding rb for Si ...
 rb = {2.416 2.416 2.416}, int_b = -4.009936231138939, err_rb = 9.936e-03
 rb = {2.899 2.899 2.899}, int_b = -3.995870951012808, err_rb = 4.129e-03
 rb = {3.382 3.382 3.382}, int_b = -4.000680453002921, err_rb = 6.805e-04
 rb = {3.866 3.866 3.866}, int_b = -3.999737866647758, err_rb = 2.621e-04
 rb = {4.349 4.349 4.349}, int_b = -4.000070550365031, err_rb = 7.055e-05
 rb = {4.832 4.832 4.832}, int_b = -4.000017751601002, err_rb = 1.775e-05
 rb = {5.315 5.315 5.315}, int_b = -3.999987293122637, err_rb = 1.271e-05
 rb = {5.798 5.798 5.798}, int_b = -4.000014504383367, err_rb = 1.450e-05
 rb = {6.281 6.281 6.281}, int_b = -4.000006710739731, err_rb = 6.711e-06
 rb = {6.765 6.765 6.765}, int_b = -4.000008429414830, err_rb = 8.429e-06
 rb = {7.248 7.248 7.248}, int_b = -4.000000440133311, err_rb = 4.401e-07
 rb = {7.731 7.731 7.731}, int_b = -4.000000010003547, err_rb = 1.000e-08
 rb = {7.731 7.731 7.731}

 ######################################################################
 Relaxation step number: 1

 Starting pseudocharge generation and self energy calculation...
 Integration b = 7.999999424940

 Integration b_ref = 8.000000000015

 ***************************************
 *          Eself_ref = 62.796570       *
 ***************************************
 Done. (0.709453 s)
 Time for b calculation: 0.810 seconds.

 Starting calculating nonlocal projectors ...
 Done. (0.142240 s)

 ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
 Starting SCF iteration...
 AAR converged to a relative residual of 1.98745e-06 in 18 iterations.
 Poisson problem took 0.087208s
 ============================================
 Relaxation iteration:  1
 SCF iteration number:  1, Chebyshev cycle: 1
 ============================================
 Fermi energy = 1.530735
 ============================================
 Relaxation iteration:  1
 SCF iteration number:  1, Chebyshev cycle: 2
 ============================================
 Fermi energy = 0.272411
 ============================================
```

```
Relaxation iteration:  1
SCF iteration number:  1, Chebyshev cycle: 3
============================================
Fermi energy = 0.182543
============================================
Relaxation iteration:  1
SCF iteration number:  1, Chebyshev cycle: 4
============================================
Fermi energy = 0.154371
------------------
Eband = -0.22804919
Exc = -3.01829174
Exc_dc = -3.16626416
Eelec_dc = 6.10670404
Eent = -0.00000000
E_corr = 0.00000270
Eself = 14.37760511
Etot = -8.35097515
------------------
Etot = -8.35097515
Eatom = -4.17548757
Error in SCF iteration: 2.3692e-01
AAR converged to a relative residual of 0.000180728 in 9 iterations.
AAR converged to a relative residual of 2.51232e-07 in 13 iterations.
Poisson problem took 0.063633s
This SCF iteration took 9.563 s.

=========================
Relaxation iteration:  1
SCF iteration number:  2
=========================
Fermi energy = 0.150575
------------------
Eband = -0.19002933
Exc = -3.03158500
Exc_dc = -3.18535995
Eelec_dc = 6.06514330
Eent = -0.00000000
E_corr = 0.00000270
Eself = 14.37760511
Etot = -8.34871350
------------------
Etot = -8.34871350
Eatom = -4.17435675
Error in SCF iteration: 1.7913e-01
AAR converged to a relative residual of 0.00021372 in 9 iterations.
AAR converged to a relative residual of 7.15562e-07 in 13 iterations.
Poisson problem took 0.067793s
This SCF iteration took 1.746 s.

=========================
Relaxation iteration:  1
SCF iteration number:  3
=========================
Fermi energy = 0.169587
------------------
Eband = -0.05433789
Exc = -3.09077821
Exc_dc = -3.26557380
Eelec_dc = 5.91570097
Eent = -0.00000000
E_corr = 0.00000270
Eself = 14.37760511
Etot = -8.34144375
```

```
------------------
Etot = -8.34144375
Eatom = -4.17072188
Error in SCF iteration: 2.2486e-02
AAR converged to a relative residual of 0.000207857 in 9 iterations.
AAR converged to a relative residual of 1.89117e-06 in 11 iterations.
Poisson problem took 0.047485s
This SCF iteration took 1.725 s.

========================
Relaxation iteration:  1
SCF iteration number:  4
========================
Fermi energy = 0.170316
------------------
Eband = -0.04864026
Exc = -3.09390696
Exc_dc = -3.26937031
Eelec_dc = 5.90907762
Eent = -0.00000000
E_corr = 0.00000270
Eself = 14.37760511
Etot = -8.34170170
------------------
Etot = -8.34170170
Eatom = -4.17085085
Error in SCF iteration: 1.7600e-02
AAR converged to a relative residual of 0.000179074 in 7 iterations.
AAR converged to a relative residual of 1.01436e-07 in 13 iterations.
Poisson problem took 0.066348s
This SCF iteration took 1.744 s.

========================
Relaxation iteration:  1
SCF iteration number:  5
========================
Fermi energy = 0.172799
------------------
Eband = -0.03024079
Exc = -3.10473836
Exc_dc = -3.28222357
Eelec_dc = 5.88812783
Eent = -0.00000000
E_corr = 0.00000270
Eself = 14.37760511
Etot = -8.34223016
------------------
Etot = -8.34223016
Eatom = -4.17111508
Error in SCF iteration: 2.2323e-03
AAR converged to a relative residual of 0.000152485 in 7 iterations.
AAR converged to a relative residual of 8.64606e-07 in 7 iterations.
Poisson problem took 0.030279s
This SCF iteration took 1.750 s.

========================
Relaxation iteration:  1
SCF iteration number:  6
========================
Fermi energy = 0.172938
------------------
Eband = -0.02922030
Exc = -3.10532856
Exc_dc = -3.28295802
```

```
Eelec_dc = 5.88695664
Eent = -0.00000000
E_corr = 0.00000270
Eself = 14.37760511
Etot = -8.34223661
------------------
Etot = -8.34223661
Eatom = -4.17111830
Error in SCF iteration: 1.6645e-03
AAR converged to a relative residual of 0.0002099 in 7 iterations.
AAR converged to a relative residual of 1.81654e-06 in 7 iterations.
Poisson problem took 0.031115s
This SCF iteration took 1.753 s.

=========================
Relaxation iteration:  1
SCF iteration number:  7
=========================
Fermi energy = 0.173086
------------------
Eband = -0.02813686
Exc = -3.10601141
Exc_dc = -3.28378507
Eelec_dc = 5.88572368
Eent = -0.00000000
E_corr = 0.00000270
Eself = 14.37760511
Etot = -8.34224193
------------------
Etot = -8.34224193
Eatom = -4.17112096
Error in SCF iteration: 3.2504e-04
AAR converged to a relative residual of 0.000219036 in 7 iterations.
AAR converged to a relative residual of 2.86468e-07 in 7 iterations.
Poisson problem took 0.038276s
This SCF iteration took 1.741 s.

=========================
Relaxation iteration:  1
SCF iteration number:  8
=========================
Fermi energy = 0.173036
------------------
Eband = -0.02848838
Exc = -3.10581490
Exc_dc = -3.28353570
Eelec_dc = 5.88612665
Eent = -0.00000000
E_corr = 0.00000270
Eself = 14.37760511
Etot = -8.34224333
------------------
Etot = -8.34224333
Eatom = -4.17112166
Error in SCF iteration: 1.7584e-04
AAR converged to a relative residual of 0.000168891 in 7 iterations.
AAR converged to a relative residual of 1.93031e-07 in 7 iterations.
Poisson problem took 0.030482s
This SCF iteration took 1.687 s.


Finished SCF iteration in 8 steps!
~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
```

```
*******************************************************
*          Energy per unit cell = -8.342243327 Ha.       *
*          Energy per atom = -4.171121663 Ha.            *
*******************************************************

Starting atomic force calculation ...
local force calculation: 0.689 s
*******************************************************
*                      Atomic Force                   *
*******************************************************
Drift free forces (Ha/Bohr):
  1.0e-04 *

 -0.531135819791003  -0.377966890174293  -0.336256522392760
  0.531135819791003   0.377966890174293   0.336256522392760

Max magnitude of forces (Ha/Bohr):     7.335071083396261e-05


Time for calculating forces: 0.837781 s.
~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
Final atomic positions (Cartesian) are as follows:
 0.000000       0.000000       0.000000
 2.562500       2.562500       2.562500

Run-time of the program: 24.243777 seconds
```

```
rmpath(MSPARC_root);
rmpath(fullfile(MSPARC_root,"src"));
rmpath("M-SPARC\");
```

Next, we run it in KSSOLV and define the cufoff energy.

```
Ecut4 = 15; % in Ha

% path and check
addpath(KSSOLV_root);
addpath("KSSOLV\");
KSSOLV_startup;
[K_cry4,K_Ham4,K_wf4,K_info4] =
kssolv_crystal(Lat_scale4,Latvec4,atom_list4,natom_list4,coord4,Ecut4,nk4);
```

```
The pseudopotential for Si is loaded from C:\Users\tvekua\OneDrive - MathWorks\Desktop\DFTMaterial\KSSOLV\/ppdata/de
Regular SCF for Pure DFT
Beging SCF4C calculation for crystal...
SCF iter   1:
eigtol =   1.000e-02
Rel Vtot Err    =            2.396e-02
Total Energy    = -7.6282487530667e+00
SCF iter   2:
eigtol =   2.995e-03
Rel Vtot Err    =            2.058e-02
Total Energy    = -7.7850168777164e+00
SCF iter   3:
eigtol =   2.573e-03
Rel Vtot Err    =            8.935e-03
Total Energy    = -7.7867378262510e+00
SCF iter   4:
eigtol =   1.117e-03
Rel Vtot Err    =            1.142e-03
```

```
Total Energy    = -7.7869758049803e+00
SCF iter   5:
eigtol =   1.427e-04
Rel Vtot Err    =            4.662e-04
Total Energy    = -7.7869769877539e+00
SCF iter   6:
eigtol =   5.828e-05
Rel Vtot Err    =            4.252e-05
Total Energy    = -7.7869777640003e+00
SCF iter   7:
eigtol =   5.316e-06
Rel Vtot Err    =            1.505e-05
Total Energy    = -7.7869777708263e+00
SCF iter   8:
eigtol =   1.881e-06
Rel Vtot Err    =            1.890e-06
Total Energy    = -7.7869777723391e+00
SCF iter   9:
eigtol =   2.362e-07
Rel Vtot Err    =            5.819e-07
Total Energy    = -7.7869777723721e+00
SCF iter  10:
eigtol =   7.273e-08
Rel Vtot Err    =            6.411e-08
Total Energy    = -7.7869777723741e+00
resnrm =   3.161e-08
resnrm =   2.018e-08
resnrm =   4.322e-08
resnrm =   4.050e-08
---------------------
resnrm =   2.694e-08
resnrm =   3.281e-08
resnrm =   2.079e-08
resnrm =   3.763e-08
---------------------
resnrm =   3.534e-08
resnrm =   2.430e-08
resnrm =   3.168e-08
resnrm =   3.436e-08
---------------------
resnrm =   2.961e-08
resnrm =   2.960e-08
resnrm =   3.174e-08
resnrm =   2.953e-08
---------------------
resnrm =   3.525e-08
resnrm =   2.408e-08
resnrm =   3.469e-08
resnrm =   3.802e-08
---------------------
resnrm =   2.952e-08
resnrm =   2.954e-08
resnrm =   3.128e-08
resnrm =   2.807e-08
---------------------
resnrm =   3.261e-08
resnrm =   3.274e-08
resnrm =   2.785e-08
resnrm =   3.409e-08
---------------------
resnrm =   2.562e-08
resnrm =   3.638e-08
resnrm =   2.410e-08
resnrm =   3.527e-08
```

```
--------------------
Etot            = -7.7869777723741e+00
Entropy         =  0.0000000000000e+00
Ekin            =  5.2031647591439e-01
Eewald          = -8.4086603810698e+00
Ealphat         =  0.0000000000000e+00
Ecor            =  1.9167405260321e+00
Ecoul           =  6.3329194366975e-01
Exc             = -2.4486663369206e+00
Efermi          =  2.4140053958911e-01
-------------------------------------
Total time used =            2.402e+01
||HX-XD||_F     =            6.168e-08
```

```
rmpath(KSSOLV_root);
rmpath("KSSOLV\");
fprintf("Total energy of the crystal from M-SPARC is %.6f Ha\n", S4.Etotal);
```

```
Total energy of the crystal from M-SPARC is -8.342243 Ha
```

```
fprintf("Atomic forces (Ha/Bohr) from M-SPARC are\n");
```

```
Atomic forces (Ha/Bohr) from M-SPARC are
```

```
for i = 1:sum(natom_list4)
    fprintf("%9.6f %9.6f %9.6f\n", S4.force(i,:));
end
```

```
-0.000053 -0.000038 -0.000034
 0.000053  0.000038  0.000034
```

```
fprintf("Total energy of the crystal from KSSOLV is %.6f Ha\n",
K_info4.Etotvec(end));
```

```
Total energy of the crystal from KSSOLV is -7.786978 Ha
```

```
fprintf("Atomic forces (Ha/Bohr) from KSSOLV are\n");
```

```
Atomic forces (Ha/Bohr) from KSSOLV are
```

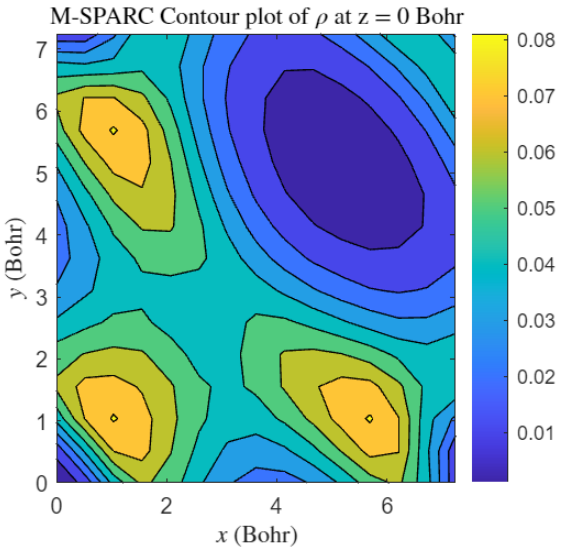
```
for i = 1:sum(natom_list4)
    fprintf("%9.6f %9.6f %9.6f\n", K_cry4.xyzforce(i,:));
end
```

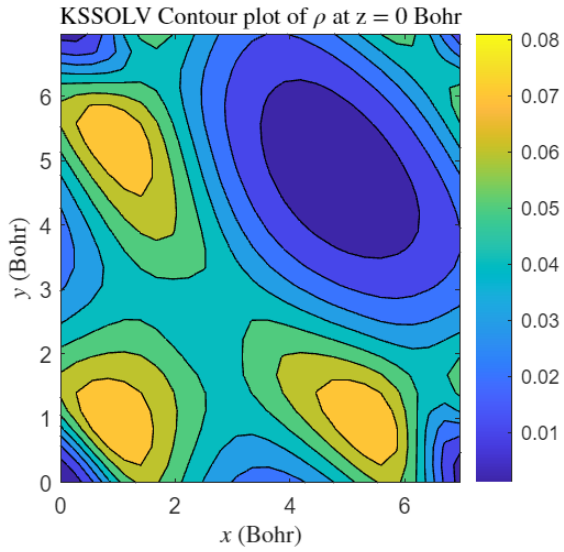
```
-0.000000  0.000000  0.000000
-0.000000 -0.000000  0.000000
```

Next we visualize the contour plot of electron density along the lattice vectors and the Density of States (DOS) plots.

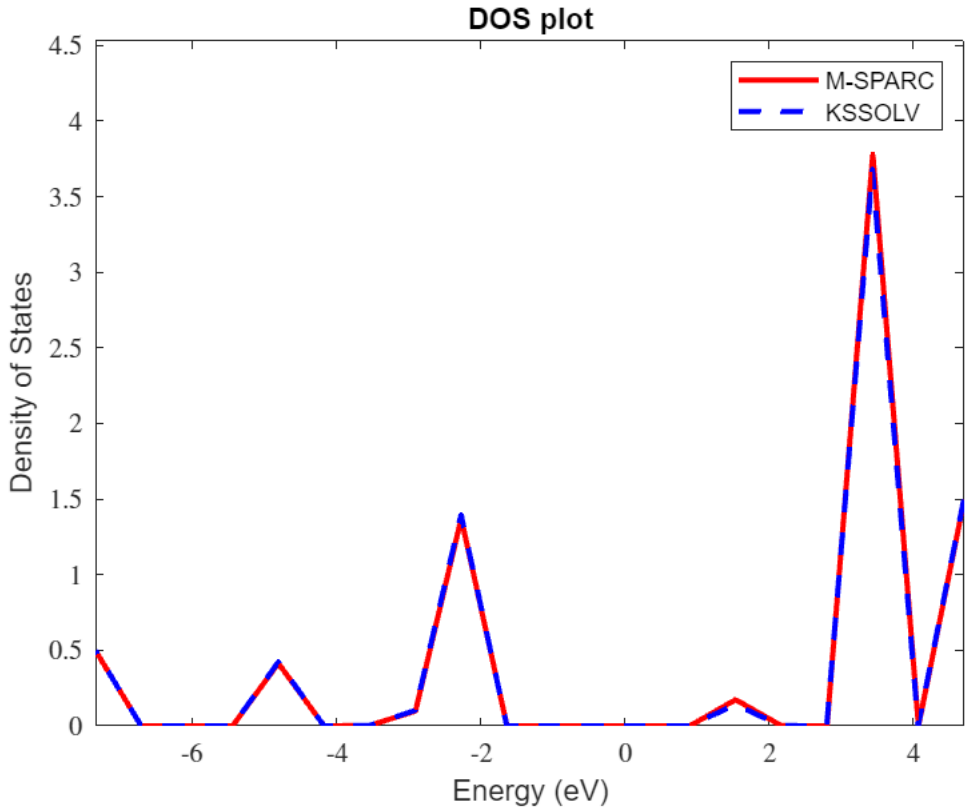
```
% M-SPARC
slice_allowed_m = string(linspace(0,S4.L1-S4.dx,S4.Nx));
zslicem = floor(double(slice_allowed_m(1))/S4.dz)+1; % in Bohr
x = linspace(0,S4.L1,S4.Nx);
y = linspace(0,S4.L2,S4.Ny);
z = linspace(0,S4.L3,S4.Nz);
[X,Y,~] = ndgrid(x,y,z);
```

```
rhom = reshape(S4.rho(:,1),[S4.Nx S4.Ny S4.Nz]);
Xm = squeeze(X(:,:,zslicem));
Ym = squeeze(Y(:,:,zslicem));
rhom = squeeze(rhom(:,:,zslicem));

% KSSOLV
L = vecnorm(K_cry4.supercell');
h = L./[K_cry4.n1;K_cry4.n2;K_cry4.n3];
slice_allowed_k = string(linspace(0,L(3)-h(3),K_cry4.n3));
zslicek = floor(double(slice_allowed_k(1))/h(3))+1; % in Bohr
x = linspace(0,L(1)-h(1),K_cry4.n1);
y = linspace(0,L(2)-h(2),K_cry4.n2);
z = linspace(0,L(3)-h(3),K_cry4.n3);
[X,Y,~] = ndgrid(x,y,z);
Xk = squeeze(X(:,:,zslicek));
Yk = squeeze(Y(:,:,zslicek));
rhok = K_Ham4.rho;
rhok = squeeze(rhok(:,:,zslicek));

fig2 = figure();
fig2.Position(3:4) = [1200, 450];
bottom = min(min(rhom(:)),min(rhok(:)));
top  = max(max(rhom(:)),max(rhok(:)));
subplot(1,2,1)
contourf(Xm,Ym,rhom)
shading interp;
colorbar
title("M-SPARC Contour plot of $\rho$ at z = "+ num2str((zslicem-1)*S4.dy,2) + "
Bohr", 'Interpreter','latex')
xlabel("$x$ (Bohr)",'Interpreter','latex')
ylabel("$y$ (Bohr)",'Interpreter','latex')
clim manual
clim([bottom top]);

subplot(1,2,2)
contourf(Xk,Yk,rhok)
shading interp;
title("KSSOLV Contour plot of $\rho$ at z = "+ num2str((zslicek-1)*h(3),2) + "
Bohr", 'Interpreter','latex')
xlabel("$x$ (Bohr)",'Interpreter','latex')
ylabel("$y$ (Bohr)",'Interpreter','latex')
clim manual
clim([bottom top]);
colorbar;
```






```
len = min(S4.Nev,max(K_wf4.ncols));
[Em_eV, DOSm_eV] = eig2DOS(S4.EigVal(1:len,:),S4.wkpt);
[Ek_eV, DOSk_eV] = eig2DOS(reshape(K_info4.Eigvals,[],K_Ham4.nkpts),K_Ham4.wks);
Ek_eV = Ek_eV - (min(Ek_eV)-min(Em_eV));
figure;
hold on; box on; hold on;
plot(Em_eV, DOSm_eV, 'r','linewidth',2,'LineStyle','-');
plot(Ek_eV, DOSk_eV, 'b','linewidth',2,'LineStyle','--');
xlim([min(Em_eV), max(Em_eV)]);
ylim([0, max(DOSm_eV(:))*1.2]);
xlabel('Energy (eV)');
ylabel('Density of States');
set(gca,'TickLabelInterpreter', 'latex');
legend("M-SPARC", "KSSOLV")
title("DOS plot")
```



2D Surfaces

We use a water surface as an example. For simulating 2D surfaces, we need to define the **Bravais lattice** as crystal. Here, we need to add a large vacuum in the Dirichlet direction to avoid the effects from periodic images. We define the Dirichlet directions below.

```
Lat_scale5 = [5.67 5.67 18.90];
Latvec5 = [1 0 0; 0 1 0; 0 0 1];
dir5 = 3;
```

Next, we define the atom symbols, number of atoms and their reduced coordinates.

```
atom_list5 = ["H","O"];
natom_list5 = [2,1];
coord5 = [ 0.7522 0.4999 0.6643; 0.2476 0.4999 0.6643; 0.4999 0.4999 0.6057];
```

Again, we define the number of k-points along preiodic directions.

```
nk5 = 2; % along each direction
```

Then we start the calculation in M-SPARC and select the mesh spacing h again.

```
h5 = 0.5; % in Bohr
```

```
addpath(MSPARC_root);
```

```
addpath(fullfile(MSPARC_root,"src"));
addpath("M-SPARC\");
% Real space toolbox M-SPARC
msparc_surface(Lat_scale5,Latvec5,atom_list5,natom_list5,coord5,dir5,h5,nk5,MSPARC_r
oot);
S5 = msparc("M-SPARC/surface");
```

```
 Reading .inpt file ...


<INPT>
# $ cat M-SPARC/surface.inpt
LATVEC_SCALE: 5.670000 5.670000 18.900000
LATVEC: 1.000000 0.000000 0.000000
 0.000000 1.000000 0.000000
 0.000000 0.000000 1.000000
MESH_SPACING: 0.500000
KPOINT_GRID: 2 2 1
KPOINT_SHIFT: 0 0 0
BC: P P D
EXCHANGE_CORRELATION: GGA_PBE
SMEARING: 1E-8
<\INPT>

 Reading .ion file ...
 Number of atom types : 2
 Total number of atoms: 3
 Default atomic mass for H is 1.007975
 Default atomic mass for O is 15.999400
 pseudo_dir # 1 = 01_H_1_1.0_1.0_pbe_v1.0.psp8
 pseudo_dir # 2 = 08_O_6_1.2_1.4_pbe_n_v1.0.psp8

 COORD:
   4.264974000000000   2.834433000000000  12.555269999999998
   1.403892000000000   2.834433000000000  12.555269999999998
   2.834433000000000   2.834433000000000  11.447730000000000

atom type 1, l = 0, r_core read 1.03328, change to rmax where |UdV| < 1E-8, 1.05000.
atom type 1, l = 1, r_core read 1.00283, change to rmax where |UdV| < 1E-8, 1.02000.
atom type 2, l = 0, r_core read 1.35246, change to rmax where |UdV| < 1E-8, 1.37000.
atom type 2, l = 1, r_core read 1.45312, change to rmax where |UdV| < 1E-8, 1.47000.
atom type 2, l = 2, r_core read 1.25127, change to rmax where |UdV| < 1E-8, 1.27000.
 reduced kpoint grid before symmetry:
                   0                   0                   0
   0.500000000000000                   0                   0
                   0   0.500000000000000                   0
   0.500000000000000   0.500000000000000                   0

 reduced kpoint grid after symmetry:
                   0                   0                   0
   0.500000000000000                   0                   0
                   0   0.500000000000000                   0
   0.500000000000000   0.500000000000000                   0

 nspin = 1, nspinor = 1, nspden = 1
## Chebyshev polynomial degree not provided, finding npl ...
## Based on the mesh size, npl is set to: 18
## Number of states not provided, finding Nev ...
## Based on the number of electrons, Nev is set to: 10
## Based on the desired accuracy, SCF_tol is set to: 2.159e-04
## Poisson tolerance not provided, choosing poisson_tol ...
## poisson_tol is set to: 2.159e-06
## Pseudocharge tolerance not provided, choosing pseudocharge_tol ...
```

```
## pseudocharge_tol is set to: 2.159e-07
 Creating differentiation matrices ...
 Done. (0.036 sec)

 Estimated memory usage:
 Total:   25.97 MB
 orbitals            :   10.28 MB
 sparse matrices     :   14.48 MB
 global-size vectors :  614.25 kB
 mixing histories    :  614.25 kB

 Finding rb for H ...
 rb = {1.890 1.989 1.989}, int_b = -0.999440013595492, err_rb = 5.600e-04
 rb = {2.362 2.487 2.487}, int_b = -1.000067349659674, err_rb = 6.735e-05
 rb = {2.835 2.984 2.984}, int_b = -1.000001170467570, err_rb = 1.170e-06
 rb = {3.308 3.482 3.482}, int_b = -0.999999966296928, err_rb = 3.370e-08
 rb = {3.308 3.482 3.482}
 Finding rb for O ...
 rb = {2.362 2.362 1.989}, int_b = -6.000051191975457, err_rb = 5.119e-05
 rb = {2.835 2.835 2.487}, int_b = -5.999855053215945, err_rb = 1.449e-04
 rb = {3.308 3.308 2.984}, int_b = -6.000038535804520, err_rb = 3.854e-05
 rb = {3.780 3.780 3.482}, int_b = -6.000014096036764, err_rb = 1.410e-05
 rb = {4.253 4.253 3.979}, int_b = -6.000024650014415, err_rb = 2.465e-05
 rb = {4.725 4.725 4.476}, int_b = -6.000024559376908, err_rb = 2.456e-05
 rb = {5.198 5.198 4.974}, int_b = -6.000019716795137, err_rb = 1.972e-05
 rb = {5.670 5.670 5.471}, int_b = -6.000015920179090, err_rb = 1.592e-05
 rb = {6.143 6.143 5.968}, int_b = -5.999998386419416, err_rb = 1.614e-06
 rb = {6.615 6.615 6.466}, int_b = -6.000000364945223, err_rb = 3.649e-07
 rb = {7.088 7.088 6.963}, int_b = -5.999999928326964, err_rb = 7.167e-08
 rb = {7.088 7.088 6.963}

 ######################################################################
 Relaxation step number: 1

 Starting pseudocharge generation and self energy calculation...
 Integration b = 8.000000204665

 Integration b_ref = 7.999999960136

 ***************************************
 *          Eself_ref = 83.183820      *
 ***************************************
 Done. (0.113990 s)
 Time for b calculation: 0.157 seconds.

 Starting calculating nonlocal projectors ...
 Done. (0.008800 s)

 ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
 Starting SCF iteration...
 AAR converged to a relative residual of 2.14216e-06 in 74 iterations.
 Poisson problem took 0.053144s
 ============================================
 Relaxation iteration:  1
 SCF iteration number:  1, Chebyshev cycle: 1
 ============================================
 Fermi energy = 0.985264
 ============================================
 Relaxation iteration:  1
 SCF iteration number:  1, Chebyshev cycle: 2
 ============================================
 Fermi energy = -0.053628
 ============================================
 Relaxation iteration:  1
```

```
 SCF iteration number:  1, Chebyshev cycle: 3
 ============================================
 Fermi energy = -0.115463
 ============================================
 Relaxation iteration:  1
 SCF iteration number:  1, Chebyshev cycle: 4
 ============================================
 Fermi energy = -0.121849
 ------------------
 Eband = -4.77556144
 Exc = -4.87328790
 Exc_dc = -5.38139750
 Eelec_dc = 13.52954336
 Eent = -0.00000000
 E_corr = -0.00056795
 Eself = 27.09112649
 Etot = -17.82960291
 ------------------
 Etot = -17.82960291
 Eatom = -5.94320097
 Error in SCF iteration: 1.1915e-01
 AAR converged to a relative residual of 1.62764e-05 in 13 iterations.

Density got negative

 AAR converged to a relative residual of 1.38028e-06 in 43 iterations.
 Poisson problem took 0.022299s
 This SCF iteration took 2.742 s.

 ========================
 Relaxation iteration:  1
 SCF iteration number:  2
 ========================
 Fermi energy = -0.122212
 ------------------
 Eband = -4.53546817
 Exc = -4.92078871
 Exc_dc = -5.44534727
 Eelec_dc = 13.28765778
 Eent = -0.00000000
 E_corr = -0.00056795
 Eself = 27.09112649
 Etot = -17.81494627
 ------------------
 Etot = -17.81494627
 Eatom = -5.93831542
 Error in SCF iteration: 8.0512e-02
 AAR converged to a relative residual of 0.000206795 in 12 iterations.

Density got negative

 AAR converged to a relative residual of 1.81782e-06 in 43 iterations.
 Poisson problem took 0.022607s
 This SCF iteration took 0.529 s.

 ========================
 Relaxation iteration:  1
 SCF iteration number:  3
 ========================
 Fermi energy = -0.120312
 ------------------
 Eband = -4.30414266
 Exc = -4.97044335
 Exc_dc = -5.51144117
```

```
 Eelec_dc = 13.04634983
 Eent = -0.00000000
 E_corr = -0.00056795
 Eself = 27.09112649
 Etot = -17.80848946
 ------------------
 Etot = -17.80848946
 Eatom = -5.93616315
 Error in SCF iteration: 4.2834e-02
 AAR converged to a relative residual of 3.12006e-05 in 13 iterations.

Density got negative

 AAR converged to a relative residual of 2.04763e-06 in 43 iterations.
 Poisson problem took 0.022350s
 This SCF iteration took 0.536 s.

 ========================
 Relaxation iteration:  1
 SCF iteration number:  4
 ========================
 Fermi energy = -0.122612
 ------------------
 Eband = -4.26451426
 Exc = -4.98195615
 Exc_dc = -5.52569699
 Eelec_dc = 13.00558515
 Eent = -0.00000000
 E_corr = -0.00056795
 Eself = 27.09112649
 Etot = -17.80688270
 ------------------
 Etot = -17.80688270
 Eatom = -5.93562757
 Error in SCF iteration: 5.7656e-03
 AAR converged to a relative residual of 4.88953e-05 in 13 iterations.

Density got negative

 AAR converged to a relative residual of 2.10952e-06 in 43 iterations.
 Poisson problem took 0.034051s
 This SCF iteration took 0.535 s.

 ========================
 Relaxation iteration:  1
 SCF iteration number:  5
 ========================
 Fermi energy = -0.123921
 ------------------
 Eband = -4.22740486
 Exc = -4.98936739
 Exc_dc = -5.53530331
 Eelec_dc = 12.96645054
 Eent = -0.00000000
 E_corr = -0.00056795
 Eself = 27.09112649
 Etot = -17.80671283
 ------------------
 Etot = -17.80671283
 Eatom = -5.93557094
 Error in SCF iteration: 5.1423e-03
 AAR converged to a relative residual of 5.00542e-05 in 13 iterations.

Density got negative
```

```
 AAR converged to a relative residual of 1.76198e-06 in 43 iterations.
 Poisson problem took 0.022378s
 This SCF iteration took 0.522 s.

 ========================
 Relaxation iteration:  1
 SCF iteration number:  6
 ========================
 Fermi energy = -0.124861
 ------------------
 Eband = -4.22841454
 Exc = -4.98692639
 Exc_dc = -5.53187147
 Eelec_dc = 12.96851423
 Eent = -0.00000000
 E_corr = -0.00056795
 Eself = 27.09112649
 Etot = -17.80664967
 ------------------
 Etot = -17.80664967
 Eatom = -5.93554989
 Error in SCF iteration: 1.8481e-03
 AAR converged to a relative residual of 3.42232e-05 in 13 iterations.

Density got negative

 AAR converged to a relative residual of 1.14891e-06 in 43 iterations.
 Poisson problem took 0.019665s
 This SCF iteration took 0.559 s.

 ========================
 Relaxation iteration:  1
 SCF iteration number:  7
 ========================
 Fermi energy = -0.123333
 ------------------
 Eband = -4.20477230
 Exc = -4.98686693
 Exc_dc = -5.53171411
 Eelec_dc = 12.94500036
 Eent = -0.00000000
 E_corr = -0.00056795
 Eself = 27.09112649
 Etot = -17.80661920
 ------------------
 Etot = -17.80661920
 Eatom = -5.93553973
 Error in SCF iteration: 6.2948e-04
 AAR converged to a relative residual of 5.3625e-05 in 13 iterations.

Density got negative

 AAR converged to a relative residual of 1.26236e-06 in 37 iterations.
 Poisson problem took 0.018782s
 This SCF iteration took 0.544 s.

 ========================
 Relaxation iteration:  1
 SCF iteration number:  8
 ========================
 Fermi energy = -0.123091
 ------------------
 Eband = -4.20009602
```

```
 Exc = -4.98679938
 Exc_dc = -5.53162587
 Eelec_dc = 12.94034192
 Eent = -0.00000000
 E_corr = -0.00056795
 Eself = 27.09112649
 Etot = -17.80662206
 ------------------
 Etot = -17.80662206
 Eatom = -5.93554069
 Error in SCF iteration: 4.8290e-04
 AAR converged to a relative residual of 3.13036e-05 in 13 iterations.

Density got negative

 AAR converged to a relative residual of 2.05323e-06 in 41 iterations.
 Poisson problem took 0.020615s
 This SCF iteration took 0.536 s.

 ========================
 Relaxation iteration:  1
 SCF iteration number:  9
 ========================
 Fermi energy = -0.122281
 ------------------
 Eband = -4.18656272
 Exc = -4.98675867
 Exc_dc = -5.53158367
 Eelec_dc = 12.92680418
 Eent = -0.00000000
 E_corr = -0.00056795
 Eself = 27.09112649
 Etot = -17.80662798
 ------------------
 Etot = -17.80662798
 Eatom = -5.93554266
 Error in SCF iteration: 2.1527e-04
 AAR converged to a relative residual of 4.81265e-05 in 13 iterations.

Density got negative

 AAR converged to a relative residual of 1.9944e-06 in 31 iterations.
 Poisson problem took 0.015099s
 This SCF iteration took 0.541 s.


 Finished SCF iteration in 9 steps!
 ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~

 ********************************************************
 *          Energy per unit cell = -17.806627979 Ha.       *
 *          Energy per atom = -5.935542660 Ha.            *
 ********************************************************

 Starting atomic force calculation ...
 local force calculation: 0.182 s
 ************************************************************
 *                      Atomic Force                        *
 ************************************************************
 Drift free forces (Ha/Bohr):
   0.000215459736965   0.000483096327607   0.020953822401891
   0.000460008450228   0.000483388005285   0.020910480434512
  -0.000675468187192  -0.000966484332892  -0.041864302836403
```

```
Max magnitude of forces (Ha/Bohr):   0.041880904971308


Time for calculating forces: 0.249335 s.
~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
Final atomic positions (Cartesian) are as follows:
 4.264974       2.834433      12.555270
 1.403892       2.834433      12.555270
 2.834433       2.834433      11.447730

Run-time of the program: 7.935370 seconds
```

```
rmpath(MSPARC_root);
rmpath(fullfile(MSPARC_root,"src"));
rmpath("M-SPARC\");
```

Next, we run it in KSSOLV and define the cufoff energy.

```
Ecut5 = 15; % in Ha

% path and check
addpath(KSSOLV_root);
addpath("KSSOLV\");
KSSOLV_startup;
[K_cry5,K_Ham5,K_w56,K_info5] =
kssolv_surface(Lat_scale5,Latvec5,atom_list5,natom_list5,coord5,dir5,Ecut5,nk5);
```

```
The pseudopotential for H is loaded from C:\Users\tvekua\OneDrive - MathWorks\Desktop\DFTMaterial\KSSOLV\/ppdata/de
The pseudopotential for O is loaded from C:\Users\tvekua\OneDrive - MathWorks\Desktop\DFTMaterial\KSSOLV\/ppdata/de
Regular SCF for Pure DFT
Beging SCF4C calculation for surface...
SCF iter   1:
eigtol =   1.000e-02
Rel Vtot Err    =            1.796e-01
Total Energy    = -1.6704243320250e+01
SCF iter   2:
eigtol =   1.000e-02
Rel Vtot Err    =            1.056e-01
Total Energy    = -1.6701448418547e+01
SCF iter   3:
eigtol =   1.000e-02
Rel Vtot Err    =            5.288e-02
Total Energy    = -1.6714283368620e+01
SCF iter   4:
eigtol =   6.610e-03
Rel Vtot Err    =            6.045e-03
Total Energy    = -1.6718064290339e+01
SCF iter   5:
eigtol =   7.556e-04
Rel Vtot Err    =            1.274e-03
Total Energy    = -1.6718128148942e+01
SCF iter   6:
eigtol =   1.593e-04
Rel Vtot Err    =            2.235e-04
Total Energy    = -1.6718128056155e+01
SCF iter   7:
eigtol =   2.793e-05
Rel Vtot Err    =            5.088e-05
Total Energy    = -1.6718128193390e+01
SCF iter   8:
```

```
eigtol =   6.360e-06
Rel Vtot Err    =            2.282e-05
Total Energy    = -1.6718128195127e+01
SCF iter   9:
eigtol =   2.852e-06
Rel Vtot Err    =            4.478e-06
Total Energy    = -1.6718128195177e+01
SCF iter  10:
eigtol =   5.598e-07
Rel Vtot Err    =            2.178e-07
Total Energy    = -1.6718128195180e+01
resnrm =   2.999e-09
resnrm =   2.889e-09
resnrm =   4.933e-09
resnrm =   3.596e-09
--------------------
resnrm =   2.244e-09
resnrm =   5.798e-09
resnrm =   3.365e-09
resnrm =   3.318e-09
--------------------
resnrm =   2.626e-09
resnrm =   2.775e-09
resnrm =   3.992e-09
resnrm =   6.562e-09
--------------------
resnrm =   2.001e-09
resnrm =   4.792e-09
resnrm =   3.236e-09
resnrm =   4.346e-09
--------------------
Etot            = -1.6718128195180e+01
Entropy         =  0.0000000000000e+00
Ekin            = -3.8076316724267e+00
Eewald          =  4.8950138654756e+00
Ealphat         =  0.0000000000000e+00
Ecor            = -3.2694514154101e+01
Ecoul           =  1.9034409175884e+01
Exc             = -4.1454054100119e+00
Efermi          = -1.7176729671863e-01
---------------------------------------
Total time used =            9.797e+00
||HX-XD||_F     =            7.505e-09
```

```
rmpath(KSSOLV_root);
rmpath("KSSOLV\");
```

```
fprintf("Total energy of the surface from M-SPARC is %.6f Ha\n", S5.Etotal);
```

```
Total energy of the surface from M-SPARC is -17.806628 Ha
```

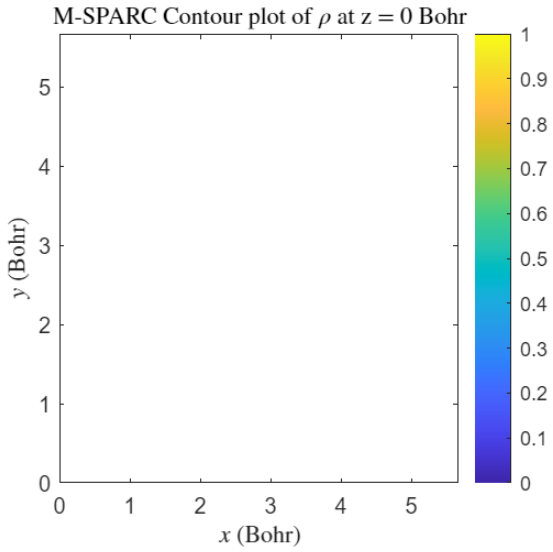
```
fprintf("Total energy of the surface from KSSOLV is %.6f Ha\n",
K_info5.Etotvec(end));
```

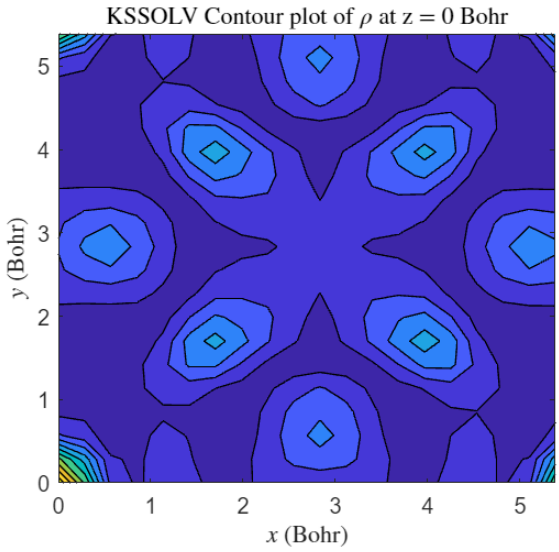
```
Total energy of the surface from KSSOLV is -16.718128 Ha
```

We visualize the electron density below. Since the pseudopotential are not identical and the number of valence electrons is different, the electron density are not the same at all.

```
% M-SPARC
```

```
slice_allowed_m = string(linspace(0,S5.L3-S5.dz,S5.Nz));
zslicem = floor(double(slice_allowed_m(1))/S5.dz)+1; % in Bohr
x = linspace(0,S5.L1,S5.Nx);
y = linspace(0,S5.L2,S5.Ny);
z = linspace(0,S5.L3,S5.Nz);
[X,Y,~] = ndgrid(x,y,z);
rhom = reshape(S5.rho(:,1),[S5.Nx S5.Ny S5.Nz]);
Xm = squeeze(X(:,:,zslicem));
Ym = squeeze(Y(:,:,zslicem));
rhom = squeeze(rhom(:,:,zslicem));

% KSSOLV
L = vecnorm(K_cry5.supercell');
h = L'./[K_cry5.n1;K_cry5.n2;K_cry5.n3];
slice_allowed_k = string(linspace(0,L(3)-h(3),K_cry5.n3));
zslicek = floor(double(slice_allowed_k(1))/h(3))+1; % in Bohr
x = linspace(0,L(1)-h(1),K_cry5.n1);
y = linspace(0,L(2)-h(2),K_cry5.n2);
z = linspace(0,L(3)-h(3),K_cry5.n3);
[X,Y,~] = ndgrid(x,y,z);
Xk = squeeze(X(:,:,zslicek));
Yk = squeeze(Y(:,:,zslicek));
rhok = K_Ham5.rho;
rhok = squeeze(rhok(:,:,zslicek));

fig2 = figure();
fig2.Position(3:4) = [1200, 450];
subplot(1,2,1)
shading interp;
colorbar
contourf(Xm,Ym,rhom)
shading interp;
colorbar
title("M-SPARC Contour plot of $\rho$ at z = "+ num2str((zslicem-1)*S5.dz,2) + "
Bohr", 'Interpreter','latex')
xlabel("$x$ (Bohr)",'Interpreter','latex')
ylabel("$y$ (Bohr)",'Interpreter','latex')

subplot(1,2,2)
contourf(Xk,Yk,rhok)
title("KSSOLV Contour plot of $\rho$ at z = "+ num2str((zslicek-1)*h(3),2) + "
Bohr", 'Interpreter','latex')
xlabel("$x$ (Bohr)",'Interpreter','latex')
ylabel("$y$ (Bohr)",'Interpreter','latex')
```





1D Wires

We use water wire (H2O) as an example. For 1D wire system, we need to define the **Bravais lattice** as crystal. Here, we need to add a large vacuum in the Dirichlet direction to avoid the effects from periodic images. And we define the periodic directions below.

```
Lat_scale6 =  [14 14 6];
Latvec6 = [1 0 0; 0 1 0; 0 0 1];
dir6 = 3;
```

Next, we define the atom symbols, numbe of atoms and their reduced coordinates.

```
atom_list6 = ["H","O"];
natom_list6 = [2,1];
coord6 = [0.52 0.5 0.74; 0.52 0.5 0.26; 0.45 0.5 0.5];
```

Again, we define the number of k-points along preiodic directions.

```
nk6 = 2; % along each direction
```

Then we start the calculation in M-SPARC and select the mesh spacing h again.

```
h6 = 0.4; % in Bohr

addpath(MSPARC_root);
addpath(fullfile(MSPARC_root,"src"));
addpath("M-SPARC\");
% Real space toolbox M-SPARC
msparc_wire(Lat_scale6,Latvec6,atom_list6,natom_list6,coord6,dir6,h6,nk6,MSPARC_root
);
S6 = msparc("M-SPARC/wire");
```

```
Reading .inpt file ...
```

```
<INPT>
# $ cat M-SPARC/wire.inpt
LATVEC_SCALE: 14.000000 14.000000 6.000000
LATVEC: 1.000000 0.000000 0.000000
 0.000000 1.000000 0.000000
 0.000000 0.000000 1.000000
MESH_SPACING: 0.400000
KPOINT_GRID: 1 1 2
KPOINT_SHIFT: 0 0 0
BC: D D P
EXCHANGE_CORRELATION: GGA_PBE
<\INPT>

 Reading .ion file ...
 Number of atom types : 2
 Total number of atoms: 3
 Default atomic mass for H is 1.007975
 Default atomic mass for O is 15.999400
 pseudo_dir # 1 = 01_H_1_1.0_1.0_pbe_v1.0.psp8
 pseudo_dir # 2 = 08_O_6_1.2_1.4_pbe_n_v1.0.psp8

 COORD:
   7.280000000000000   7.000000000000000   4.440000000000000
   7.280000000000000   7.000000000000000   1.560000000000000
   6.300000000000000   7.000000000000000   3.000000000000000

atom type 1, l = 0, r_core read 1.03328, change to rmax where |UdV| < 1E-8, 1.05000.
atom type 1, l = 1, r_core read 1.00283, change to rmax where |UdV| < 1E-8, 1.02000.
atom type 2, l = 0, r_core read 1.35246, change to rmax where |UdV| < 1E-8, 1.37000.
atom type 2, l = 1, r_core read 1.45312, change to rmax where |UdV| < 1E-8, 1.47000.
atom type 2, l = 2, r_core read 1.25127, change to rmax where |UdV| < 1E-8, 1.27000.
 reduced kpoint grid before symmetry:
                   0                   0                   0
                   0                   0   0.500000000000000

 reduced kpoint grid after symmetry:
                   0                   0                   0
                   0                   0   0.500000000000000

 nspin = 1, nspinor = 1, nspden = 1
## Chebyshev polynomial degree not provided, finding npl ...
## Based on the mesh size, npl is set to: 20
## Number of states not provided, finding Nev ...
## Based on the number of electrons, Nev is set to: 10
## Based on the desired accuracy, SCF_tol is set to: 2.159e-04
## Poisson tolerance not provided, choosing poisson_tol ...
## poisson_tol is set to: 2.159e-06
## Pseudocharge tolerance not provided, choosing pseudocharge_tol ...
## pseudocharge_tol is set to: 2.159e-07
 Creating differentiation matrices ...
 Done. (0.080 sec)

 Estimated memory usage:
 Total:   72.08 MB
 orbitals            :   17.80 MB
 sparse matrices     :   50.13 MB
 global-size vectors :    2.08 MB
 mixing histories    :    2.08 MB

 Finding rb for H ...
 rb = {1.600 1.600 1.600}, int_b = -0.999561152213818, err_rb = 4.388e-04
 rb = {2.000 2.000 2.000}, int_b = -1.000034585129104, err_rb = 3.459e-05
 rb = {2.400 2.400 2.400}, int_b = -1.000034585129104, err_rb = 3.459e-05
```

```
rb = {2.800 2.800 2.800}, int_b = -1.000016194121715, err_rb = 1.619e-05
rb = {3.200 3.200 3.200}, int_b = -1.000003672492823, err_rb = 3.672e-06
rb = {3.600 3.600 3.600}, int_b = -0.999999551081521, err_rb = 4.489e-07
rb = {4.000 4.000 4.000}, int_b = -1.000000094617160, err_rb = 9.462e-08
rb = {4.000 4.000 4.000}
Finding rb for O ...
rb = {2.000 2.000 2.000}, int_b = -5.999463035463749, err_rb = 5.370e-04
rb = {2.400 2.400 2.400}, int_b = -5.999463035463749, err_rb = 5.370e-04
rb = {2.800 2.800 2.800}, int_b = -6.000013291767375, err_rb = 1.329e-05
rb = {3.200 3.200 3.200}, int_b = -6.000028253891916, err_rb = 2.825e-05
rb = {3.600 3.600 3.600}, int_b = -6.000009177804044, err_rb = 9.178e-06
rb = {4.000 4.000 4.000}, int_b = -6.000013054369730, err_rb = 1.305e-05
rb = {4.400 4.400 4.400}, int_b = -6.000020703077120, err_rb = 2.070e-05
rb = {4.800 4.800 4.800}, int_b = -6.000025365855456, err_rb = 2.537e-05
rb = {5.200 5.200 5.200}, int_b = -6.000021395999332, err_rb = 2.140e-05
rb = {5.600 5.600 5.600}, int_b = -6.000020457529147, err_rb = 2.046e-05
rb = {6.000 6.000 6.000}, int_b = -5.999997318522845, err_rb = 2.681e-06
rb = {6.400 6.400 6.400}, int_b = -6.000000557478126, err_rb = 5.575e-07
rb = {6.800 6.800 6.800}, int_b = -5.999999890524674, err_rb = 1.095e-07
rb = {6.800 6.800 6.800}

###################################################################
Relaxation step number: 1

Starting pseudocharge generation and self energy calculation...
WARNING: Atom 3 too close to boundary for b calculation
WARNING: Atom 3 too close to boundary for b calculation
WARNING: Atom 3 too close to boundary for b calculation
Integration b = 8.000000145942

Integration b_ref = 8.000000000016

**************************************
*          Eself_ref = 62.080566       *
**************************************
Done. (0.099443 s)
Time for b calculation: 0.128 seconds.

Starting calculating nonlocal projectors ...
Done. (0.009287 s)

~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
Starting SCF iteration...
AAR converged to a relative residual of 1.00975e-06 in 61 iterations.
Poisson problem took 0.191946s
===========================================
Relaxation iteration:  1
SCF iteration number:  1, Chebyshev cycle: 1
===========================================
Fermi energy = 1.451793
===========================================
Relaxation iteration:  1
SCF iteration number:  1, Chebyshev cycle: 2
===========================================
Fermi energy = 0.144907
===========================================
Relaxation iteration:  1
SCF iteration number:  1, Chebyshev cycle: 3
===========================================
Fermi energy = -0.081231
===========================================
Relaxation iteration:  1
SCF iteration number:  1, Chebyshev cycle: 4
===========================================
```

```
 Fermi energy = -0.108595
 ------------------
 Eband = -4.97420330
 Exc = -4.76999849
 Exc_dc = -5.44034024
 Eelec_dc = 13.42881723
 Eent = -0.00000000
 E_corr = -0.00022325
 Eself = 26.84670253
 Etot = -17.72197010
 ------------------
 Etot = -17.72197010
 Eatom = -5.90732337
 Error in SCF iteration: 1.2990e-01
 AAR converged to a relative residual of 7.79185e-05 in 13 iterations.

Density got negative

 AAR converged to a relative residual of 2.05639e-06 in 38 iterations.
 Poisson problem took 0.123372s
 This SCF iteration took 3.918 s.

 ========================
 Relaxation iteration:  1
 SCF iteration number:  2
 ========================
 Fermi energy = -0.108431
 ------------------
 Eband = -4.65177508
 Exc = -4.83663898
 Exc_dc = -5.52624020
 Eelec_dc = 13.11111916
 Eent = -0.00000000
 E_corr = -0.00022325
 Eself = 26.84670253
 Etot = -17.69798047
 ------------------
 Etot = -17.69798047
 Eatom = -5.89932682
 Error in SCF iteration: 7.8694e-02
 AAR converged to a relative residual of 7.05037e-05 in 13 iterations.

Density got negative

 AAR converged to a relative residual of 1.47287e-06 in 37 iterations.
 Poisson problem took 0.121227s
 This SCF iteration took 0.913 s.

 ========================
 Relaxation iteration:  1
 SCF iteration number:  3
 ========================
 Fermi energy = -0.105997
 ------------------
 Eband = -4.39775732
 Exc = -4.89291362
 Exc_dc = -5.59939888
 Eelec_dc = 12.84847468
 Eent = -0.00000000
 E_corr = -0.00022325
 Eself = 26.84670253
 Etot = -17.68972315
 ------------------
 Etot = -17.68972315
```

```
 Eatom = -5.89657438
 Error in SCF iteration: 4.4455e-02
 AAR converged to a relative residual of 0.000134551 in 14 iterations.

Density got negative

 AAR converged to a relative residual of 5.89513e-07 in 43 iterations.
 Poisson problem took 0.127945s
 This SCF iteration took 0.976 s.

 ========================
 Relaxation iteration:  1
 SCF iteration number:  4
 ========================
 Fermi energy = -0.106720
 ------------------
 Eband = -4.35330074
 Exc = -4.90771919
 Exc_dc = -5.62011864
 Eelec_dc = 12.80007142
 Eent = -0.00000000
 E_corr = -0.00022325
 Eself = 26.84670253
 Etot = -17.68775565
 ------------------
 Etot = -17.68775565
 Eatom = -5.89591855
 Error in SCF iteration: 7.7496e-03
 AAR converged to a relative residual of 0.000143346 in 15 iterations.

Density got negative

 AAR converged to a relative residual of 5.91977e-07 in 37 iterations.
 Poisson problem took 0.135697s
 This SCF iteration took 1.013 s.

 ========================
 Relaxation iteration:  1
 SCF iteration number:  5
 ========================
 Fermi energy = -0.106829
 ------------------
 Eband = -4.31720451
 Exc = -4.91700502
 Exc_dc = -5.63200424
 Eelec_dc = 12.76136879
 Eent = -0.00000000
 E_corr = -0.00022325
 Eself = 26.84670253
 Etot = -17.68776227
 ------------------
 Etot = -17.68776227
 Eatom = -5.89592076
 Error in SCF iteration: 5.6276e-03
 AAR converged to a relative residual of 0.000151798 in 14 iterations.

Density got negative

 AAR converged to a relative residual of 6.03455e-07 in 37 iterations.
 Poisson problem took 0.133382s
 This SCF iteration took 0.935 s.

 ========================
 Relaxation iteration:  1
```

```
 SCF iteration number:  6
 ========================
 Fermi energy = -0.107871
 ------------------
 Eband = -4.32603423
 Exc = -4.91538769
 Exc_dc = -5.62974103
 Eelec_dc = 12.77078568
 Eent = -0.00000000
 E_corr = -0.00022325
 Eself = 26.84670253
 Etot = -17.68782098
 ------------------
 Etot = -17.68782098
 Eatom = -5.89594033
 Error in SCF iteration: 1.7079e-03
 AAR converged to a relative residual of 0.000155205 in 15 iterations.

Density got negative

 AAR converged to a relative residual of 2.03619e-06 in 32 iterations.
 Poisson problem took 0.109002s
 This SCF iteration took 0.911 s.

 ========================
 Relaxation iteration:  1
 SCF iteration number:  7
 ========================
 Fermi energy = -0.107246
 ------------------
 Eband = -4.31478524
 Exc = -4.91658586
 Exc_dc = -5.63133166
 Eelec_dc = 12.75915173
 Eent = -0.00000000
 E_corr = -0.00022325
 Eself = 26.84670253
 Etot = -17.68781349
 ------------------
 Etot = -17.68781349
 Eatom = -5.89593783
 Error in SCF iteration: 1.1333e-03
 AAR converged to a relative residual of 0.000154319 in 15 iterations.

Density got negative

 AAR converged to a relative residual of 2.15287e-06 in 35 iterations.
 Poisson problem took 0.111932s
 This SCF iteration took 0.881 s.

 ========================
 Relaxation iteration:  1
 SCF iteration number:  8
 ========================
 Fermi energy = -0.106715
 ------------------
 Eband = -4.30809238
 Exc = -4.91644834
 Exc_dc = -5.63115718
 Eelec_dc = 12.75248190
 Eent = -0.00000000
 E_corr = -0.00022325
 Eself = 26.84670253
 Etot = -17.68782743
```

```
 ------------------
 Etot = -17.68782743
 Eatom = -5.89594248
 Error in SCF iteration: 5.4892e-04
 AAR converged to a relative residual of 0.000133955 in 14 iterations.

Density got negative

 AAR converged to a relative residual of 6.4048e-07 in 37 iterations.
 Poisson problem took 0.117199s
 This SCF iteration took 1.020 s.

 ========================
 Relaxation iteration:  1
 SCF iteration number:  9
 ========================
 Fermi energy = -0.105769
 ------------------
 Eband = -4.29761898
 Exc = -4.91679042
 Exc_dc = -5.63159780
 Eelec_dc = 12.74184287
 Eent = -0.00000000
 E_corr = -0.00022325
 Eself = 26.84670253
 Etot = -17.68789451
 ------------------
 Etot = -17.68789451
 Eatom = -5.89596484
 Error in SCF iteration: 2.3252e-04
 AAR converged to a relative residual of 0.000146031 in 16 iterations.

Density got negative

 AAR converged to a relative residual of 9.80757e-07 in 31 iterations.
 Poisson problem took 0.112820s
 This SCF iteration took 0.880 s.

 ========================
 Relaxation iteration:  1
 SCF iteration number: 10
 ========================
 Fermi energy = -0.105429
 ------------------
 Eband = -4.29618883
 Exc = -4.91669743
 Exc_dc = -5.63146109
 Eelec_dc = 12.74044225
 Eent = -0.00000000
 E_corr = -0.00022325
 Eself = 26.84670253
 Etot = -17.68790869
 ------------------
 Etot = -17.68790869
 Eatom = -5.89596956
 Error in SCF iteration: 1.0264e-04
 AAR converged to a relative residual of 0.000122708 in 13 iterations.

Density got negative

 AAR converged to a relative residual of 2.03394e-06 in 20 iterations.
 Poisson problem took 0.079574s
 This SCF iteration took 0.889 s.
```

```
Finished SCF iteration in 10 steps!
~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~

*******************************************************
*          Energy per unit cell = -17.687908691 Ha.       *
*          Energy per atom = -5.895969564 Ha.             *
*******************************************************

Starting atomic force calculation ...
WARNING: Atom 3 too close to boundary for b calculation
WARNING: Atom 3 too close to boundary for b calculation
WARNING: Atom 3 too close to boundary for b calculation
local force calculation: 0.124 s
*******************************************************
*                      Atomic Force                   *
*******************************************************
Drift free forces (Ha/Bohr):
  0.044531320398341  -0.000000886961346   0.021332152639668
  0.044531170116461  -0.000000823372800  -0.021337619136110
 -0.089062490514802   0.000001710334146   0.000005466496442

Max magnitude of forces (Ha/Bohr):   0.089062490698986


Time for calculating forces: 0.202747 s.
~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
Final atomic positions (Cartesian) are as follows:
 7.280000       7.000000       4.440000
 7.280000       7.000000       1.560000
 6.300000       7.000000       3.000000

Run-time of the program: 13.221379 seconds
```

```
rmpath(MSPARC_root);
rmpath(fullfile(MSPARC_root,"src"));
rmpath("M-SPARC\");
```

Next, we run it in KSSOLV and define the cufoff energy.

```
Ecut6 = 15; % in Ha

% path and check
addpath(KSSOLV_root);
addpath("KSSOLV\");
KSSOLV_startup;
[K_cry6,K_Ham6,K_wf6,K_info6] =
kssolv_surface(Lat_scale6,Latvec6,atom_list6,natom_list6,coord6,dir6,Ecut6,nk6);
```

```
The pseudopotential for H is loaded from C:\Users\tvekua\OneDrive - MathWorks\Desktop\DFTMaterial\KSSOLV\/ppdata/de
The pseudopotential for O is loaded from C:\Users\tvekua\OneDrive - MathWorks\Desktop\DFTMaterial\KSSOLV\/ppdata/de
Regular SCF for Pure DFT
Beging SCF4C calculation for surface...
SCF iter   1:
eigtol =   1.000e-02
Rel Vtot Err    =            1.612e-01
Total Energy    = -1.6703673105271e+01
SCF iter   2:
eigtol =   1.000e-02
Rel Vtot Err    =            8.348e-02
```

```
Total Energy    = -1.6699322777553e+01
SCF iter   3:
eigtol =   1.000e-02
Rel Vtot Err    =            5.223e-02
Total Energy    = -1.6712194316704e+01
SCF iter   4:
eigtol =   6.529e-03
Rel Vtot Err    =            8.080e-03
Total Energy    = -1.6720021504056e+01
SCF iter   5:
eigtol =   1.010e-03
Rel Vtot Err    =            4.941e-03
Total Energy    = -1.6720039105092e+01
SCF iter   6:
eigtol =   6.176e-04
Rel Vtot Err    =            8.835e-04
Total Energy    = -1.6720046138372e+01
SCF iter   7:
eigtol =   1.104e-04
Rel Vtot Err    =            4.666e-04
Total Energy    = -1.6720046192459e+01
SCF iter   8:
eigtol =   5.833e-05
Rel Vtot Err    =            1.015e-04
Total Energy    = -1.6720046192981e+01
SCF iter   9:
eigtol =   1.268e-05
Rel Vtot Err    =            3.328e-05
Total Energy    = -1.6720046193429e+01
SCF iter  10:
eigtol =   4.161e-06
Rel Vtot Err    =            9.132e-06
Total Energy    = -1.6720046193427e+01
resnrm =   7.185e-07
resnrm =   8.125e-07
resnrm =   8.449e-07
resnrm =   8.615e-07
---------------------
resnrm =   7.199e-07
resnrm =   8.124e-07
resnrm =   8.440e-07
resnrm =   8.613e-07
---------------------
resnrm =   7.190e-07
resnrm =   8.123e-07
resnrm =   8.446e-07
resnrm =   8.614e-07
---------------------
resnrm =   7.204e-07
resnrm =   8.122e-07
resnrm =   8.439e-07
resnrm =   8.611e-07
---------------------
Etot            = -1.6720046193427e+01
Entropy         =  0.0000000000000e+00
Ekin            = -4.2084321723538e+00
Eewald          =  1.4131265307431e+00
Ealphat         =  0.0000000000000e+00
Ecor            = -2.4915787733384e+01
Ecoul           =  1.5159988798184e+01
Exc             = -4.1689416166167e+00
Efermi          = -2.6934097379897e-01
--------------------------------------
```

```
Total time used =           2.169e+01
||HX-XD||_F     =           1.622e-06
```

```
rmpath(KSSOLV_root);
rmpath("KSSOLV\");
```

```
fprintf("Total energy of the wire from M-SPARC is %.6f Ha\n", S6.Etotal);
```

```
Total energy of the wire from M-SPARC is -17.687909 Ha
```

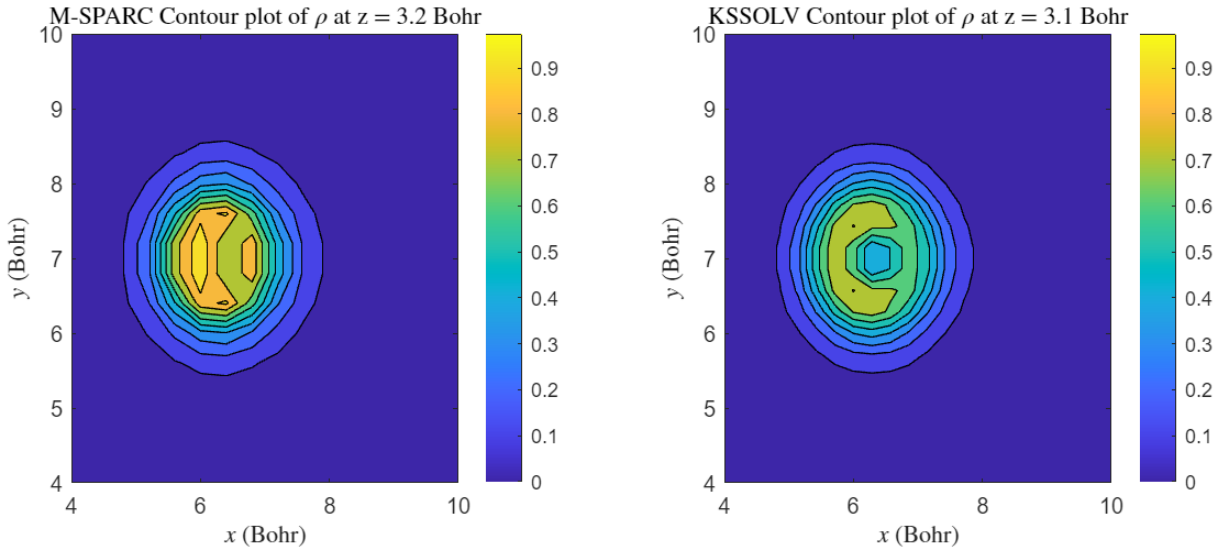
```
fprintf("Total energy of the wire from KSSOLV is %.6f Ha\n", K_info6.Etotvec(end));
```

```
Total energy of the wire from KSSOLV is -16.720046 Ha
```

We visualize the electron density below. Since the pseudopotentials are not identical and the number of valence electrons is different, the visualized electron densities from the two toolboxes are quite different from each other.

```
% M-SPARC
slice_allowed_m = string(linspace(0,S6.L3-S6.dz,S6.Nz));
zslicem = floor(double(slice_allowed_m(9))/S6.dz)+1; % in Bohr
x = linspace(0,S6.L1,S6.Nx);
y = linspace(0,S6.L2,S6.Ny);
z = linspace(0,S6.L3,S6.Nz);
[X,Y,~] = ndgrid(x,y,z);
rhom = reshape(S6.rho(:,1),[S6.Nx S6.Ny S6.Nz]);
Xm = squeeze(X(:,:,zslicem));
Ym = squeeze(Y(:,:,zslicem));
rhom = squeeze(rhom(:,:,zslicem));

% KSSOLV
L = vecnorm(K_cry6.supercell');
h = L'./[K_cry6.n1;K_cry6.n2;K_cry6.n3];
slice_allowed_k = string(linspace(0,L(3)-h(3),K_cry6.n3));
zslicek = floor(double(slice_allowed_k(12))/h(3))+1; % in Bohr
x = linspace(0,L(1)-h(1),K_cry6.n1);
y = linspace(0,L(2)-h(2),K_cry6.n2);
z = linspace(0,L(3)-h(3),K_cry6.n3);
[X,Y,Z] = ndgrid(x,y,z);
Xk = squeeze(X(:,:,zslicek));
Yk = squeeze(Y(:,:,zslicek));
rhok = K_Ham6.rho;
rhok = squeeze(rhok(:,:,zslicek));

bottom = min(min(rhom(:)),min(rhok(:)));
top  = max(max(rhom(:)),max(rhok(:)));
fig2 = figure();
fig2.Position(3:4) = [1200, 450];
subplot(1,2,1)
contourf(Xm,Ym,rhom)
shading interp;
colorbar
```

```
title("M-SPARC Contour plot of $\rho$ at z = "+ num2str((zslicem-1)*S6.dy,2) + "
Bohr", 'Interpreter','latex')
xlabel("$x$ (Bohr)",'Interpreter','latex')
ylabel("$y$ (Bohr)",'Interpreter','latex')
xlim([4 10])
ylim([4 10])
clim manual
clim([bottom top]);

subplot(1,2,2)
contourf(Xk,Yk,rhok)
shading interp;
colorbar
title("KSSOLV Contour plot of $\rho$ at z = "+ num2str((zslicek-1)*h(3),2) + "
Bohr", 'Interpreter','latex')
xlabel("$x$ (Bohr)",'Interpreter','latex')
ylabel("$y$ (Bohr)",'Interpreter','latex')
xlim([4 10])
ylim([4 10])
clim manual
clim([bottom top]);
colorbar;
```



Functions

```
function [E_eV, DOS_eV] = eig2DOS(lambda1,wkpt)
% plot Density Of States (DOS)
eV2Ha = 1 / 27.21138397;
% Plot DOS in eV
% convert lambda to eV
lambda1_eV = lambda1 / eV2Ha;
nkpts = size(lambda1_eV,2);
assert(length(wkpt) == nkpts);
assert(sum(wkpt) == 1);
```

```
mu = 0.1; % in eV
N = 5 * size(lambda1_eV,1);
lambda_max = max(max(lambda1_eV));
lambda_min = min(min(lambda1_eV));

for kpt = 1:nkpts
    [DOS_eV_temp1,E_eV] = eig2DOS_gamma(lambda1_eV(:,kpt), N, mu, lambda_max,
lambda_min);

    if kpt==1
        DOS_eV = DOS_eV_temp1*wkpt(1);
    else
        DOS_eV = DOS_eV + DOS_eV_temp1*wkpt(kpt);
    end
end
end

function [DOS, E] = eig2DOS_gamma(lambda,N,sigma,lambda_min,lambda_max)
% EIG2DOS plots density of states (DOS) based on the eigenvalues
% DOE(e) = 2 \sum_{n=1}^{Ns} delta(lambda(n) -  e)
%
% @param lambda Eigenvalues
% @param n      Number of points in E
% @param sigma  Standard deviation
%
% @author       Qimen Xu <qimenxu@gatech.edu>

buf = 0;
Emin = lambda_min - buf;
Emax = lambda_max + buf;
E = linspace(Emin, Emax, N);
DOS = sum(gauss_distribution(colminusrow(E, lambda), sigma), 2);
end

function f = gauss_distribution(x, s)
% f(x,mu,s) = 1/(s*sqrt(2*pi)) * exp( -0.5 * ((x)/s)^2 )
p1 = -.5 * ((x)./s) .^ 2;
p2 = (s * sqrt(2*pi));
f = exp(p1) ./ p2;
end

% tool function colminusrow
function xmy = colminusrow(x,y)
% A column vector x minus a row vector.
% In Matlab versions after R2018b, it's just x - y
[xx,yy] = ndgrid(x,y);
xmy = xx - yy;
end
```