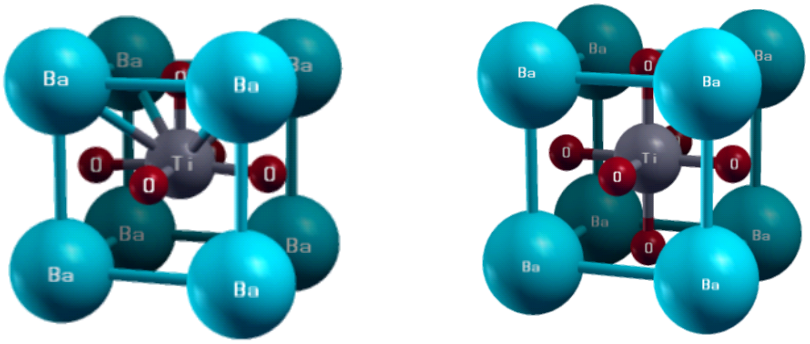
Tutorial 1: Spontaneous polarization in $BaTiO_3$ (approx. 20 mins)

For the calculation of spontaneous polarization of $BaTiO_3$ two structures has been chosen. One is tetragonal non-centrosymmetric (lambda1), where the atoms were displaced from the equilibrium centrosymmetric positions in Z direction, and another structure is a centrosymmetric structure (lambda0).



1 Case lambda1 (non-centrosymmetric)

We begin with the non-centrosymmetric structure, since it has the lowest symmetry.

1.0 Copy the tutorial files to your local directory

```
$ cp -r ~/group/tutorials-BerryPI/tutorial1 ~/tutorials-BerryPI/tutorial1
```

1.1 Change the current directory to `~/tutorials-BerryPI/tutorial1/lambda1`

1.2 Perform WIEN2k initialization

```
$ init_lapw -b -vxc 13 -ecut -6 -numk 230 -rkmax 6
```

Here "-vxc 13" stands for PBE-GGA as the exchange correlation functional."-ecut -6" means the separation energy of -6 Ry has been chosen to separate core electron from valance electron. “-numk 230" means that 230 k points has been chosen in Brillouin zone which generates 6ξ6ξ6 size k-mesh in the symmetric Brillouin zone. "-rkmax 6" indicates that the product between the smallest muffin tin radius and the K_max was chosen as 6 for tutorial purposes.

1.3 Execute WIEN2k SCF calculation in order to obtain the self-consistent electron density.

```
$ run_lapw
```

Important: Do not use iterative diagonalization (-it switch) during the SCF cycle. This can lead to

incorrect polarization value.

1.4 Run BerryPI

```
$ berrypi -p$(pwd) -k6:6:6
```

Here "-p$(pwd)" means that BerryPI program is running for the case (BaTiO3) located in the current directory. "-k6:6:6" means the calculation is being done using 6ξ6ξ6 k-mesh in the full Brillouin zone with a total of 216 k points.

Note: k-mesh in BerryPI should not necessarily be identical to that used in the SCF cycle

1.5 Once the calculation is completed take a note of the polarization values

```
       ---POLARIZATION IN C/m^2 FOR [0 to 2] PHASE/2PI RANGE---

TOTAL POLARIZATION: [ _____________ , _____________ , _____________]

      ---POLARIZATION IN C/m^2 FOR [-1 to +1] PHASE/2PI RANGE---

TOTAL POLARIZATION: [ _____________ , _____________ , _____________]
```

Here three total polarization values corresponds to X, Y and Z components of polarization, respectively.

Note: The total polarization has been reported twice for different pi wrapping approaches.

2 Case lambda0

The atoms are brought in centrosymmetric arrangement in order to compare its polarization with the non-centrosymmetric structure.

2.1 Copy all files from lambda1 to lambda0 directory

```
$ cp * ../lambda0
```

2.2 Change the current directory to lambda0

```
$ cd ../lambda0
```

2.3 Remove the `lambda1.struct` file.

```
$ rm lambda1.struct
```

2.4 Rename all `lambda1.*` files to `lambda0.*` files with

```
$ rename_files lambda1 lambda0
```

2.5 Restore original k-mesh taking into account the symmetry

```
$ x kgen
```

with 230 k-points (shifted)

2.6 Initialize the electron density according to the new structure

```
$ x dstart
```

2.7 Run standard SCF cycle.

```
$ run_lapw
```

2.8 Run BerryPI

```
$ berrypi -p$(pwd) -k6:6:6
```

2.9 Once the calculation is completed the results will be printed like this

```
       ---POLARIZATION IN C/m^2 FOR [0 to 2] PHASE/2PI RANGE---
TOTAL POLARIZATION: [ _____________ , _____________ , _____________]
      ---POLARIZATION IN C/m^2 FOR [-1 to +1] PHASE/2PI RANGE---
TOTAL POLARIZATION: [ _____________ , _____________ , _____________]
```

3 Spontaneous polarization

Calculation of Spontaneous Polarization using the Z components of polarizations obtained in lambda1 and lambda0.The spontaneous polarization is defined as the difference in the polarization between the centrosymmetric (lambda1) and non-centrosymmetric (lambda0) structures.

```
P_s= P_z(lambda1)- P_z(lambda0)=
_____________ - ____________ = _____________ C/m^2
```

Check whether the different π -wrappings affect the result? Here only Z components of polarization is considered because the atoms in non-centrosymmetric structure are displaced only in Z direction relative to the centrosymmetric structure

The obtained spontaneous polarization value can be compared to the experimental spontaneous polarization of 0.26 C/m^2 [1] and other DFT values of 0.22- 0.29 C/m^2 [2-3].

[1] H.H. Wieder Phys. Rev., 99 (1955), p. 1161
[2] M. Fechner, S. Ostanin, I. Mertig Phys. Rev. B, 77 (2008), p. 094112
[3] J.J. Wang, F.Y. Meng, X.Q. Ma, M.X. Xu, L.Q. Chen J. Appl. Phys., 108 (2010), p. 034107