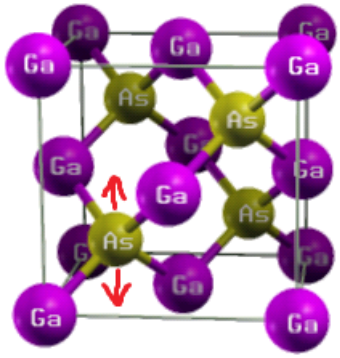
Tutorial 2: Born effective charges in GaAs (approx. 30 mins)

For the calculation of Born effective charge of As in GaAs one of the 4 As atoms has been displaced along Z-axis form its equilibrium position by +0.01(lambda1) and -0.01(lambda2) in fractional coordinates.



1 Case lambda1

In this case our structure is 8-atom zinc blende cell with one As atom displaced by +0.01 (fractional coordinate) in Z direction from its equilibrium position. Here we compute the total Berry phase (sum of electronic and ionic phase) for this structure.

1.0 Copy the tutorial files to your local directory

```
$ cp -r ~/group/tutorials-BerryPI/tutorial2 ~/tutorials-BerryPI/tutorial2
```

1.1 Change the current directory to `~/tutorials-BerryPI/tutorial2/lambda1`

1.2 Perform WIEN2k initialization

```
$ init_lapw -b -vxc 13 -ecut -6 -numk 30 -rkmax 5
```

Here "-vxc 13" stands for PBE-GGA as exchange correlation function."-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 Brillouion zone which generates 6*6*6 size k-mesh in the symmetric Brillouion zone. "-rkmax 5" indicates that the product between the smallest muffin tin radius and the K_max was chosen as 5 (this can be a bit too low for a "well converged" calculation).

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

```
$ run_lapw
```

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

1.4 Run BerryPI

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

Here "-p$(pwd)" means that BerryPI program is running for the case (GaAs) 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 the result will be printed like this

```
                ---PHASES/2*PI IN [0 to 2]RANGE---

TOTAL PHASE/(2*PI): [ _____________ , _____________ , _____________ ]

                ---PHASES/2*PI IN [-1 to +1]RANGE---

TOTAL PHASE/(2*PI): [ _____________ , _____________ , _____________ ]
```

Here three total phase (sum of electronic and ionic phase) values correspond to X, Y and Z components of total phase, respectively. As the structure has only been perturbed in Z direction, only Z component of total phase will be considered further.

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

2 Case lambda2

Calculation of the total phase (sum of electronic and ionic phase) for a state where the As atom has been displaced by -0.01 (fractional coordinate) in Z direction from its equilibrium position.

2.1 Copy all files from `lambda1` to `lambda2` directory

```
$ cp * ../lambda2
```

2.2 Change the current directory to `lambda2`

```
$ cd ../lambda2
```

2.3 Remove the `lambda1.struct` file.

```
$ rm lambda1.struct
```

2.4 Rename all `lambda1.*` files to `lambda2.*` files

```
$ rename_files lambda1 lambda2
```

2.5 Restore original k-mesh taking into account the symmetry

```
$ x kgen
```

with 30 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

```
                ---PHASES/2*PI IN [0 to 2]RANGE---

TOTAL PHASE/(2*PI): [ _____________ , _____________ , _____________ ]

                ---PHASES/2*PI IN [-1 to +1]RANGE---

TOTAL PHASE/(2*PI): [ _____________ , _____________ , _____________ ]
```

3. Born effective charge

Now let us determine the Born effective charge of As using Z component of the total phase obtained for lambda1 and lambda2 cases. The Born effective charge (in units of the elementary charge) is defined as

$$Z^*_{ZZ} = \frac{1}{2\pi} \frac{d\,\Phi_Z}{d\,u_Z}$$

Where, Z^*_{ZZ} is the born effective charge in Z direction for applied perturbation in Z direction.

$d\,\Phi_Z$ is a difference in the total phase between the two structure (do not forget 2π), and $d\,u_Z$ is the relative displacement of the particular atom (in fractional coordinates)

$$Z^*_{ZZ} = \frac{1}{2\pi} \frac{\Phi_Z(\lambda_1) - \Phi_Z(\lambda_2)}{u_Z(\lambda_1) - u_Z(\lambda_2)} \;=$$

Warning: When calculating the difference in total phase between two structures, one has to be careful about pi wrapping artifact. Draw a unit circle in order to visualize phases. Then it becomes apparent which values to take for $\Phi_Z(\lambda_1) - \Phi_Z(\lambda_2)$.

What does the sign of Z^* mean? What do you think should be the value of Z^*_{ZZ} for Ga? How does the magnitude of Z^* relate to element's valency?

Compare your result with experimental value of -2.18 [1] and also with DFT value of -2.00 [2].

[1] G. S. Spencer, A. C. Ho, J. Nenendez, R. Droopad, H. Fathollahnejad and G. N. Maracas, Phys. Rev. B 50, 14125 (1994)

[2] T. Sengstag, N. Binggeli, A. Baldereschi Phys. Rev. B, 52 (1995), p. R8613