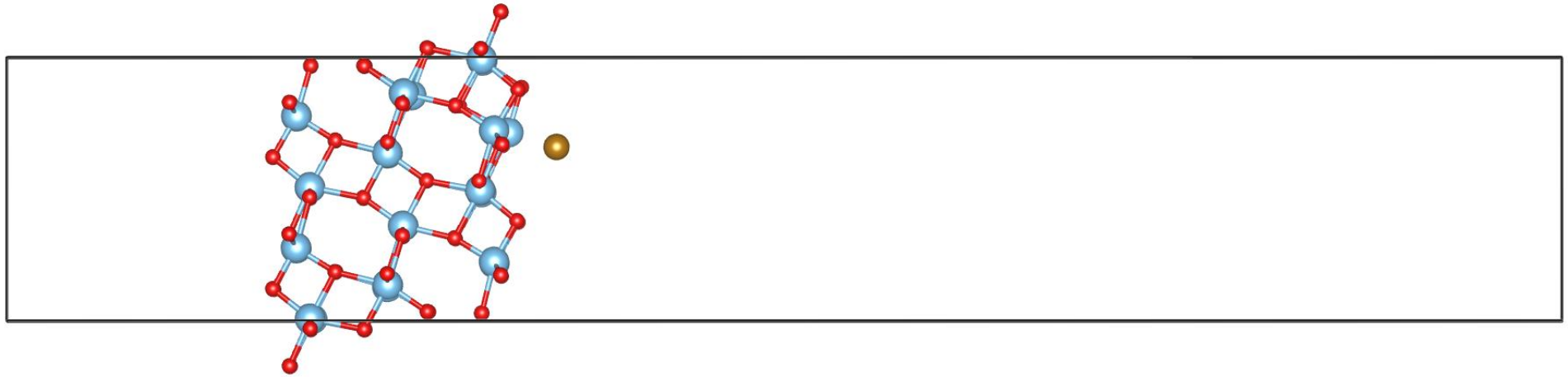
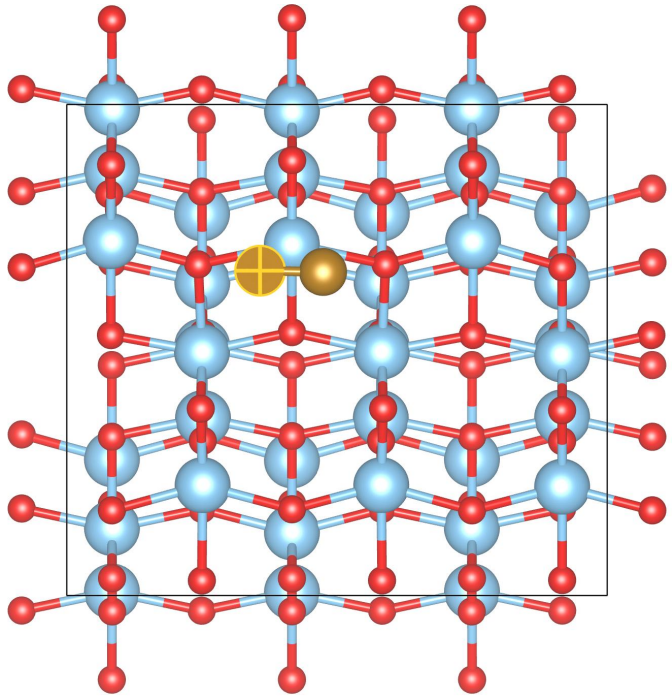
Hands on 3

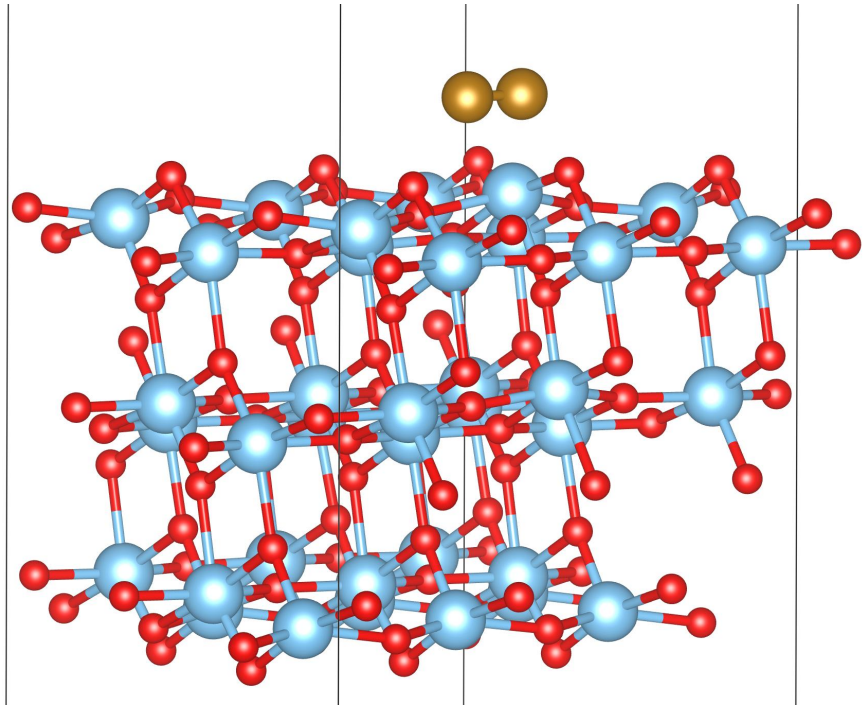
$O_2^-.TiO_2$ Potential Bending & Ghost States

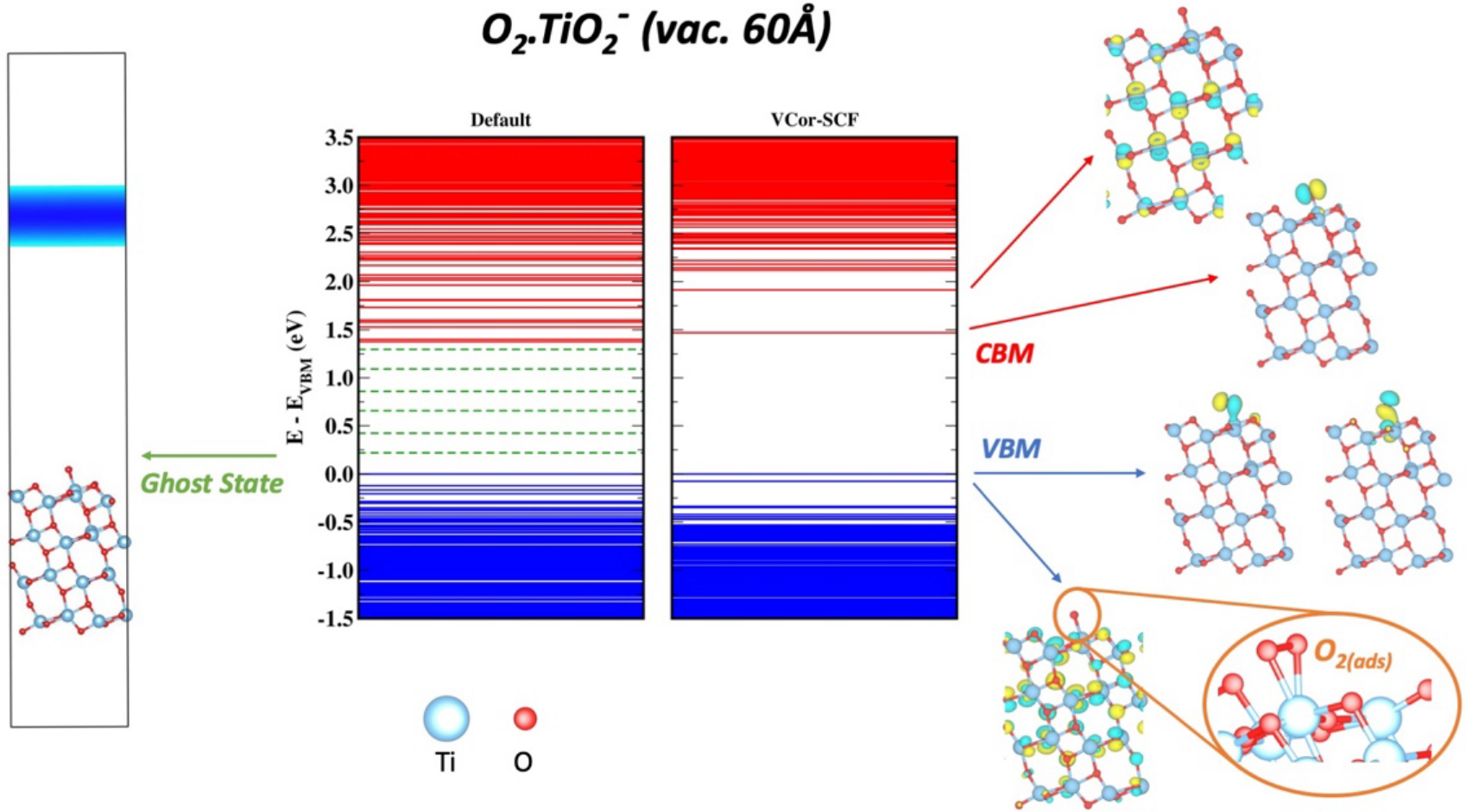
Additional Requirements

- ***Python3***
- ***GnuPlot***








$O_2.TiO_2^-$ (vac. 60Å)
Default
VCor-SCF
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
E - E$_{VBM}$ (eV)
Ghost State
CBM
VBM
$O_{2(ads)}$
Ti
O

O2tio2 Folder

- CHARGED: default charged system
- FIGURE : figure generation
- NEUTRAL : default neutral system to be used as reference
- SAVE : initial guess using the charged system
- SCPC-1: our correction

Default calculation

- Run with the default calculation the CHARGED, NEUTRAL and SAVE
- SAVE is the same of CHARGED but with EDIFF = larger just to start the convergence
- We are going to use the SAVE/CHGCAR and SAVE/WAVECAR for starting the SCPC-1

SAVE INCAR

```
# Functional Definition
  GGA = PE ;
  LREAL = Auto ;
  ENCUT = 150.00 ;
  EDIFF = 5.0E-2 ; default 1.0E-4, this is just for initial guess
```

- The use of the converged CHGCAR and WAVECAR from the uncorrected charged system Cannot be used when you have ghost states
- You can start the SCPC method from the scratch but it is not efficient
- The procedure is to run a calculation on the charged system but with few step just to start the convergence and use the WAVECAR and the CHGCAR from this calculation.
- Only SCPC-1 charge model was able to fix the ghost states

SCPC-1

```
#SCPC
  DOVCOR   =  T
  INVCOR   =  1
  VCQTOT   = -1.00
  VCZLOW   =  0.15
  VCZHIG   =  0.34
  VCDIEL   =  6.68
  VCBROAD  =  0.70
#
```

- Copy the NEUTRAL/CHGCAR ➔ REFCHG
- Copy the NEUTRAL/LOCPOT ➔ LOCPOT
- Copy the SAVE/CHGCAR ➔ CHGCAR
- Copy the SAVE/WAVECAR ➔ WAVECAR

INCAR SCPC-1

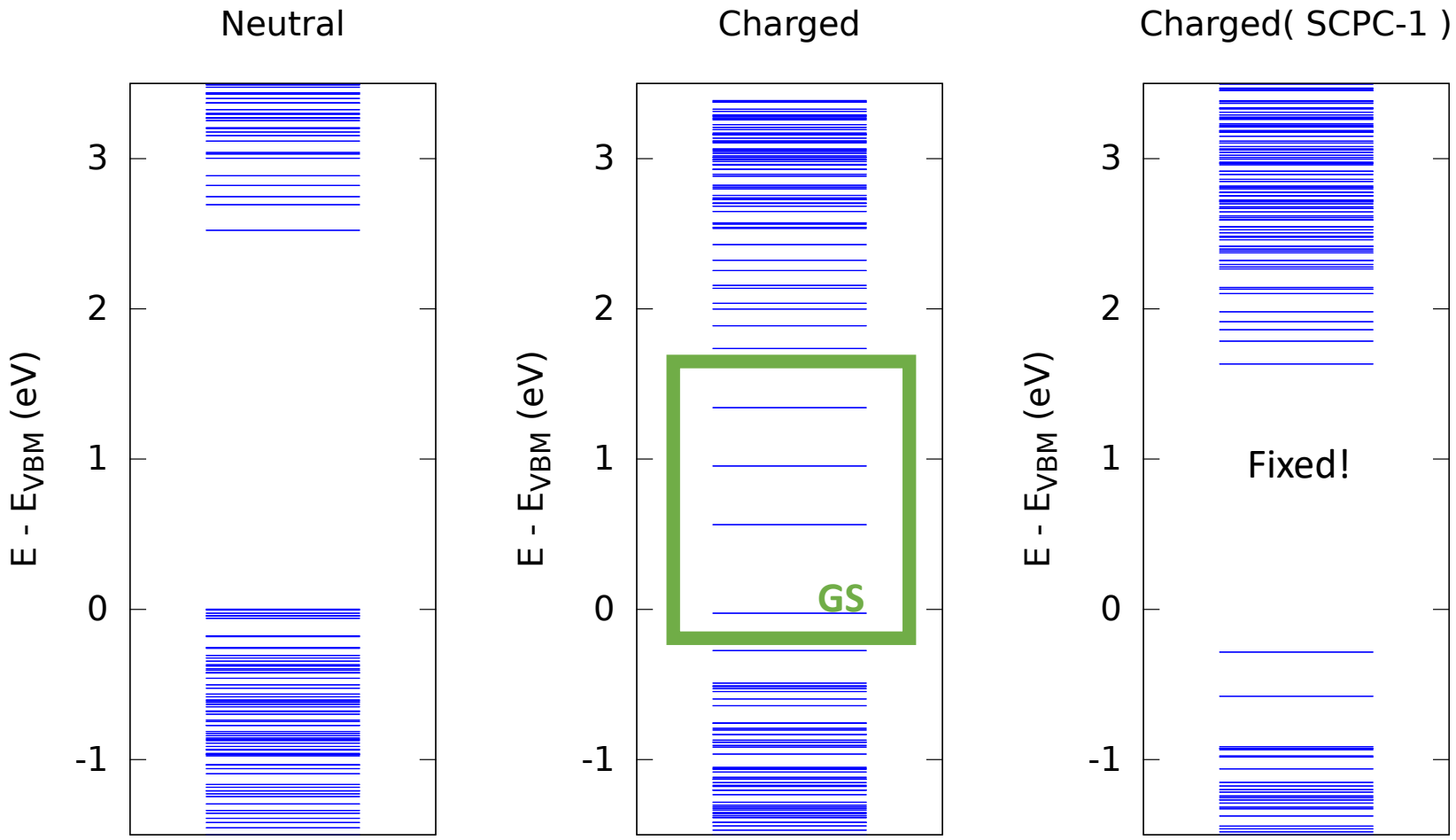
```
# Initial Guess
ISTART = 1 ;
ICHARG = 1 ;
```

```
#SCPC
  DOVCOR    =  T
  INVCOR    =  1
  VCQTOT    = -1.00
  VCZLOW    =  0.15
  VCZHIG    =  0.34
  VCDIEL    =  6.68
  VCBROAD   =  0.70
#
```

Generating the Final figures (Results)

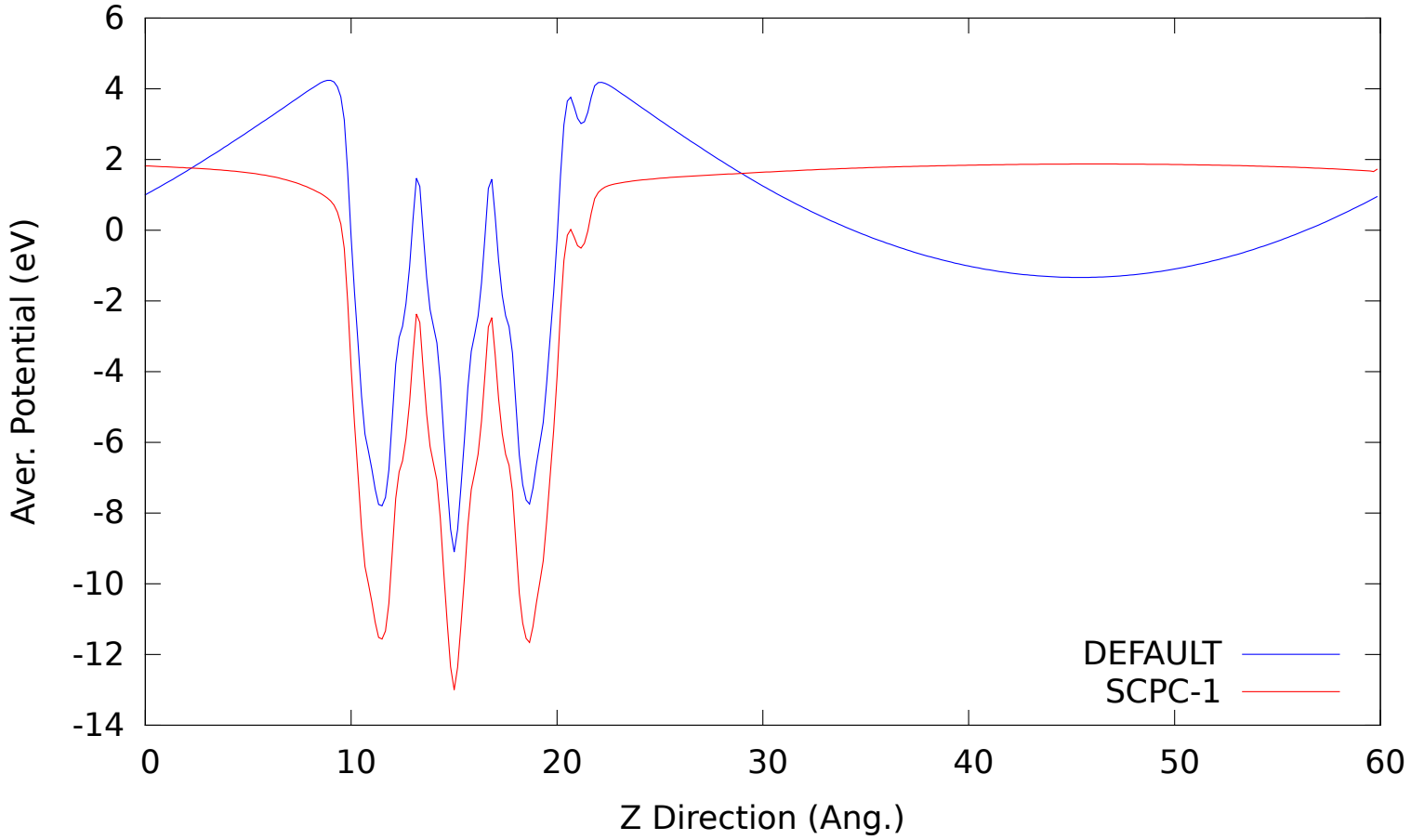
- Go to the FIGURE folder
- Run the script Check
- The Figure pdf files should be created

Eigenstates



GS: ghost states

Electrostatic Potential



- It is a negative defect.
- Part of the negative charge migrates to the middle of the vacuum due to the abnormal periodic charge interactions.
- This unphysical situation causes a bending in the electrostatic potential in the middle of the vacuum.
- With the SCPC-1 we can correct the potential.
- This is a demonstration calculation, it is not fully converged !!!