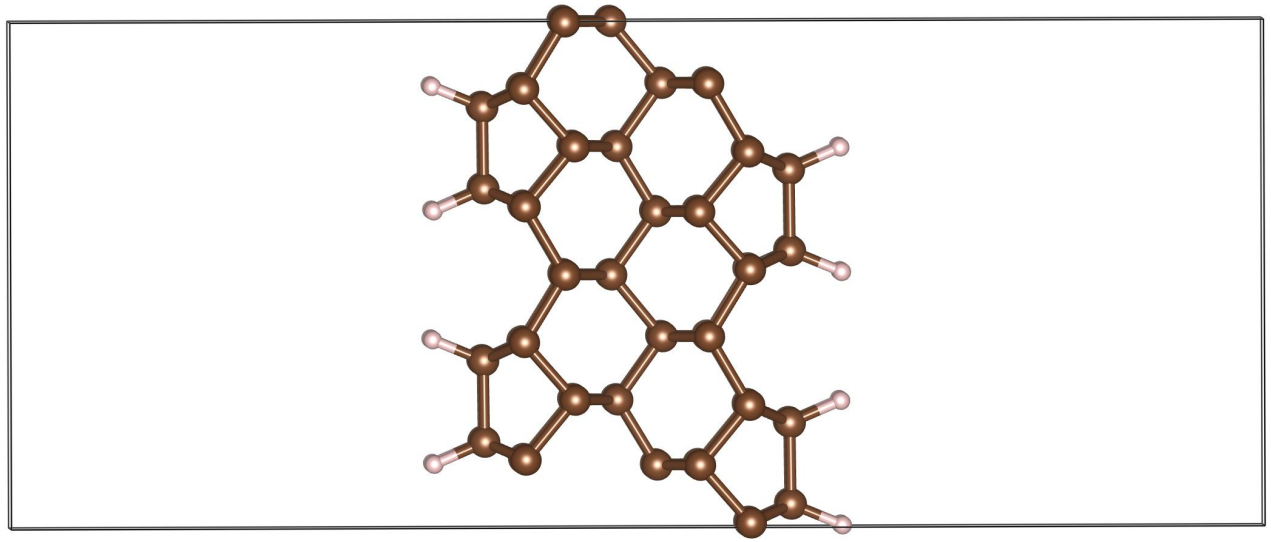
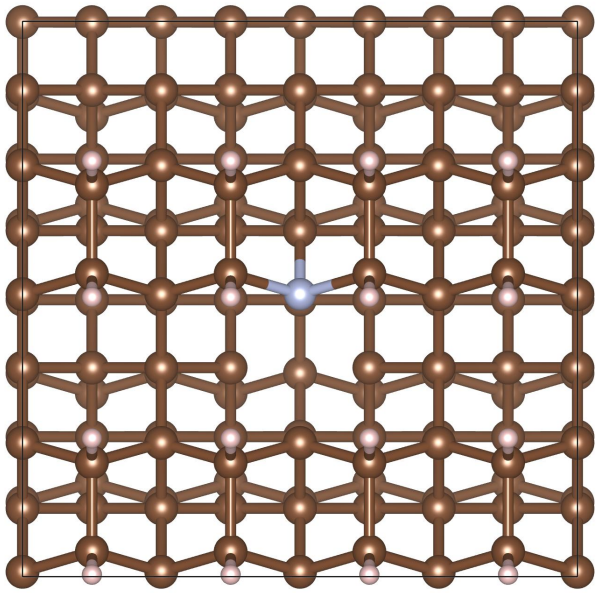
Hands on 4

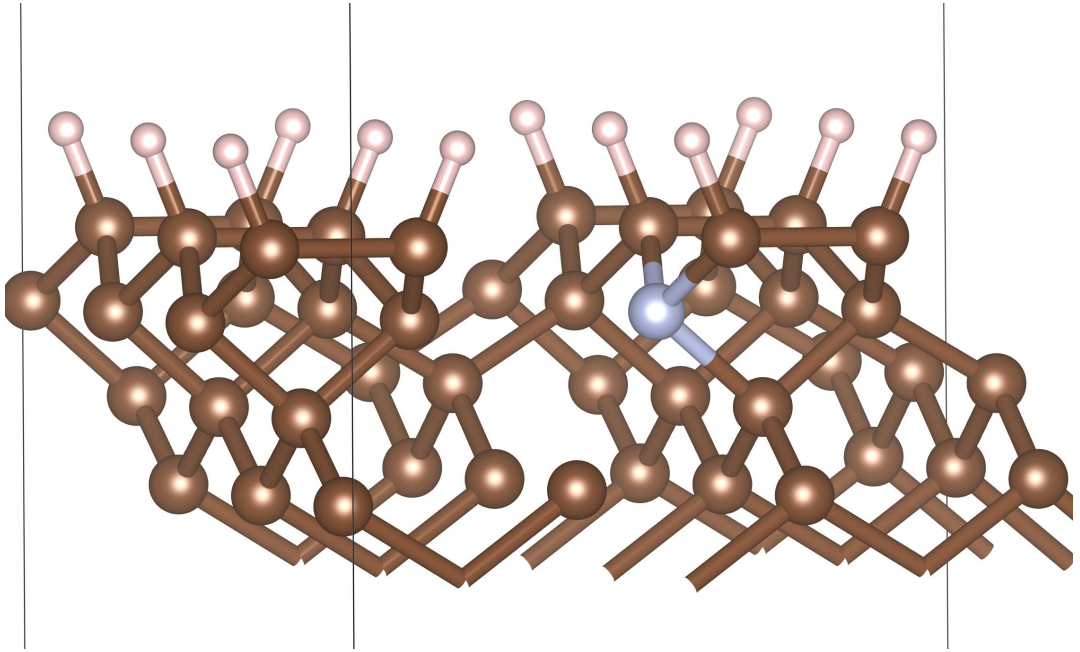
Band Structure of $N_cV_c^-$ at hydrogenated diamond 100 slab

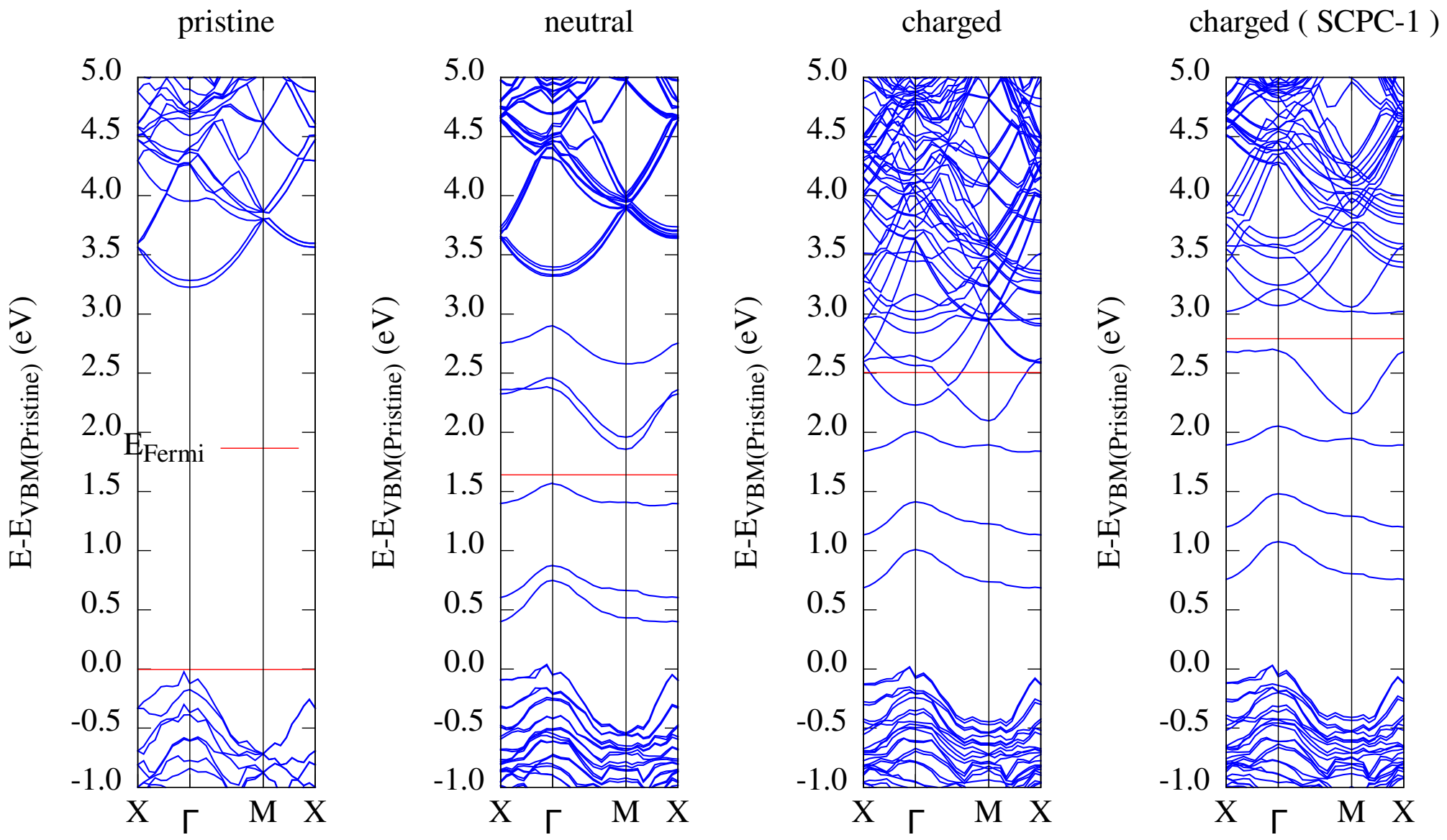
Additional Requirements

- ***Python3***
- ***Pyprocar library***



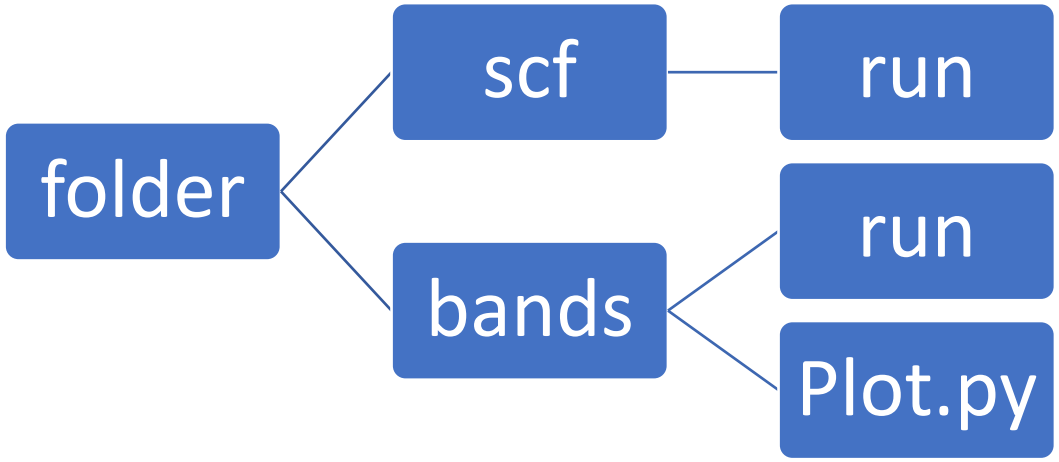





pristine
neutral
charged
charged (SCPC-1)
E-E$_{VBM(Pristine)}$ (eV)
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
E$_{Fermi}$
X
Γ
M
X

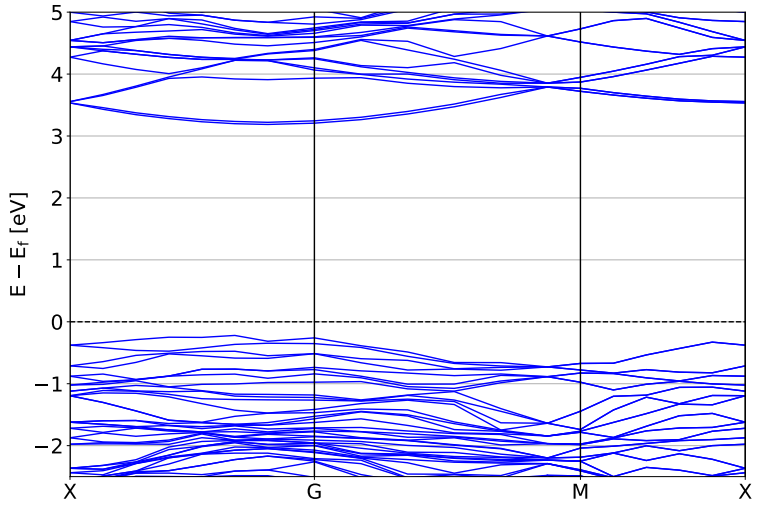
Folder

- 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



RUN

SCF → BANDS → plot.py



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

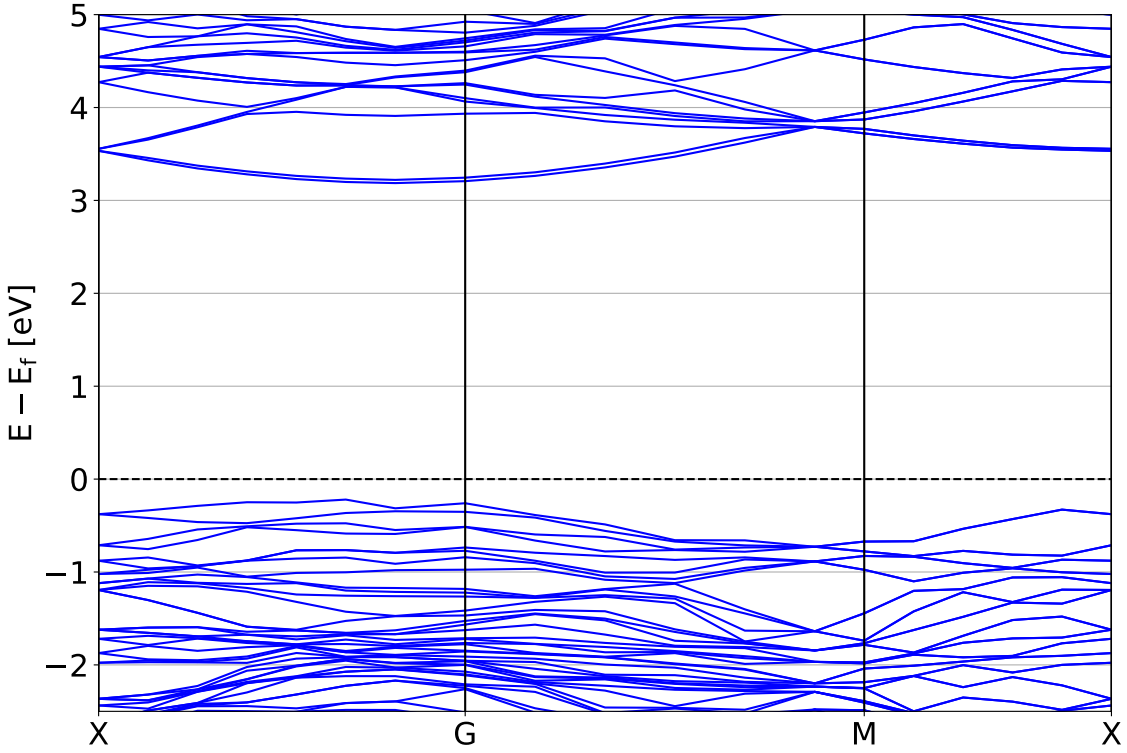
- Copy the NEUTRAL/CHGCAR → REFCHG
- Copy the NEUTRAL/LOCPOT → LOCPOT
- Copy the SAVE/CHGCAR → CHGCAR
- Copy the SAVE/WAVECAR → WAVECAR

INCAR SCPC-1

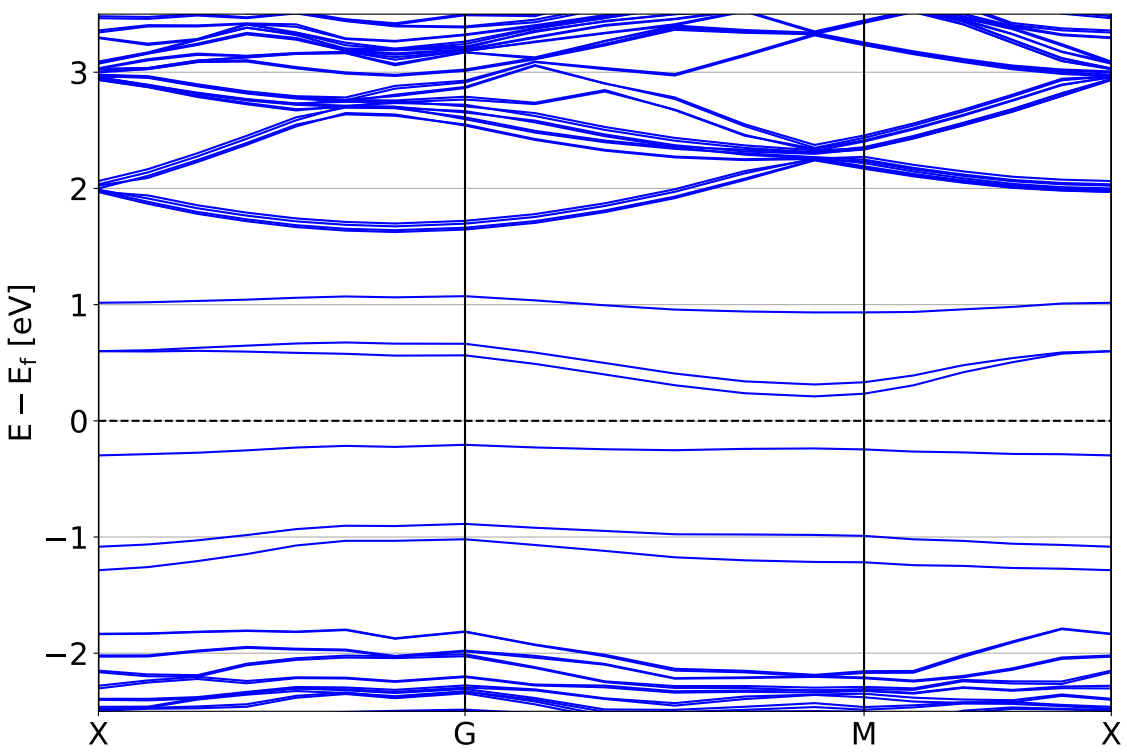
 # Initial Guess
ISTART = 1 ;
ICHARG = 1 ;

```
#SCPC ;
  DOVCOR  =  T    ;
  INVCOR  =  1    ;
  VCQTOT  = -1.00 ;
  VCZLOW  =  0.33 ;
  VCZHIG  =  0.66 ;
  VCBROAD =  0.10 ;
  VCDIEL  =  5.85 ;
  VCRXCUT =  0.15 ;
  VCRYCUT =  0.15 ;
#
```

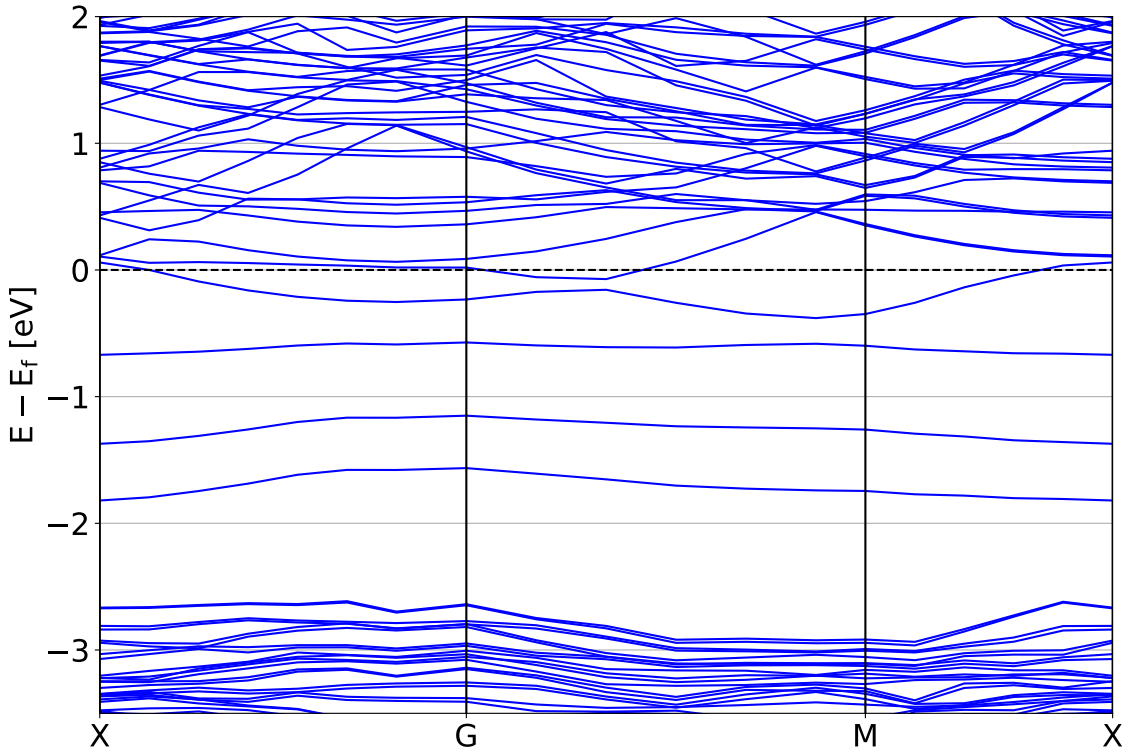
Pristine



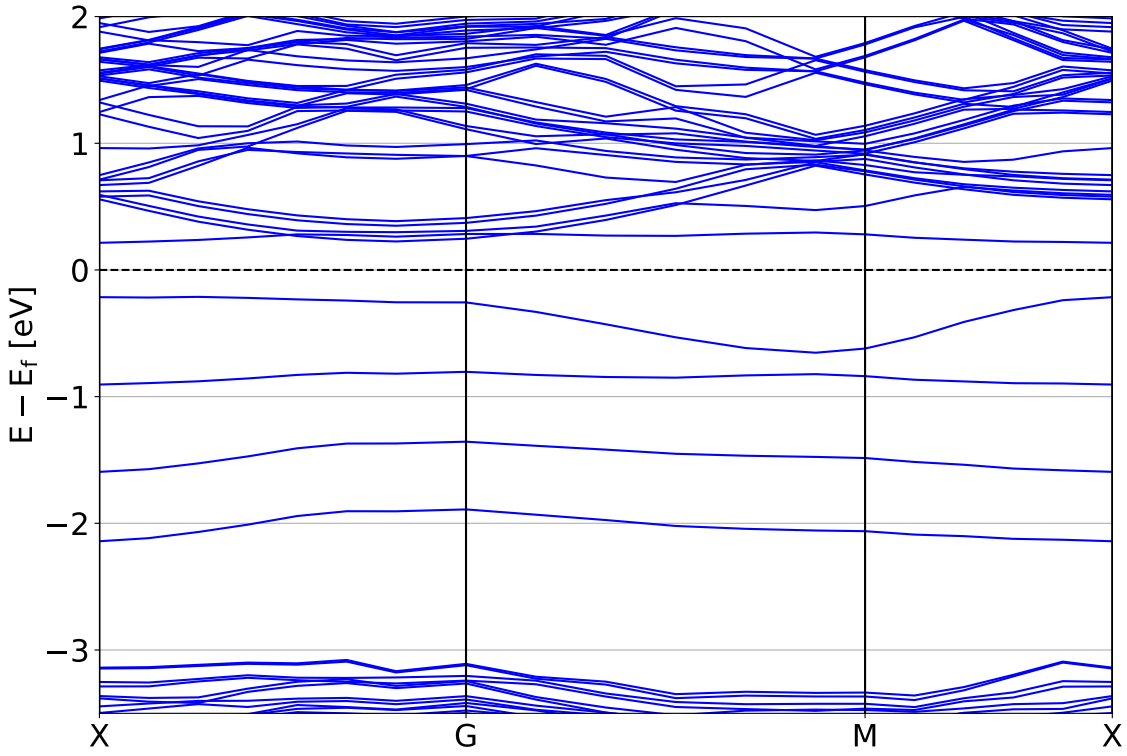
Neutral Defect



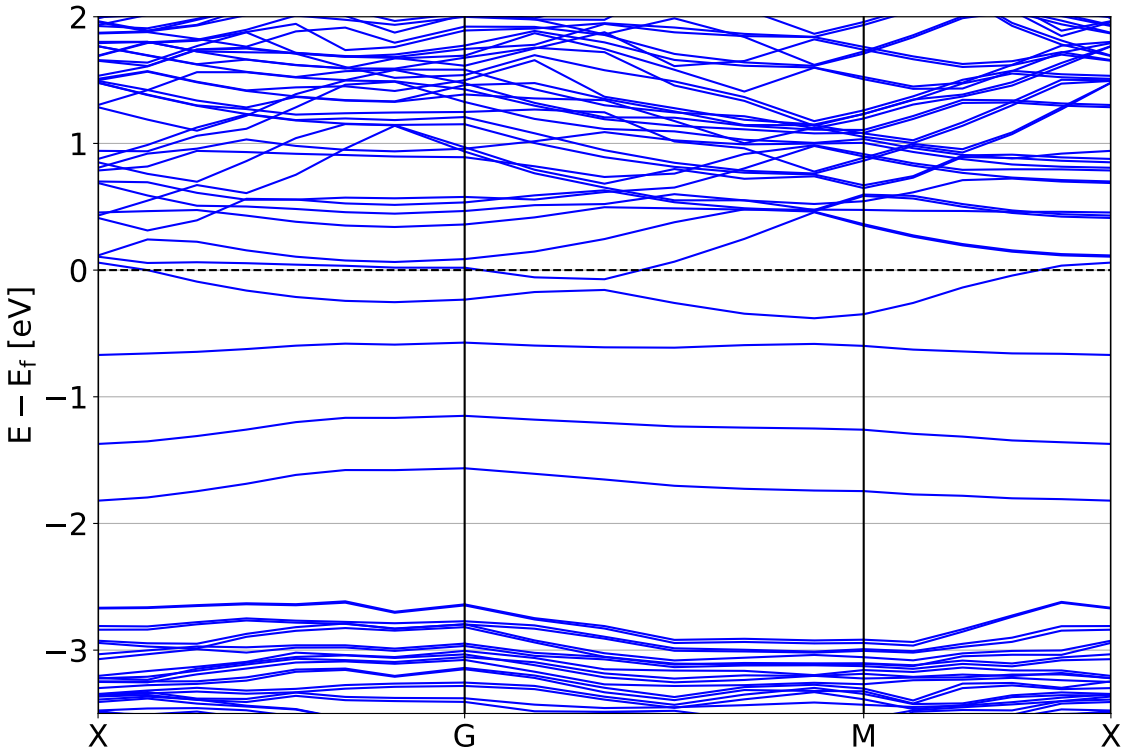
Uncorrected Charged System



Corrected SCPC-1



Charged default



SCPC-1