Hands on 2

Vc(2-) at bulk diamond

V_C^{2-} Formation Energy

$$E_f(V_C^{2-}) = E_{charged} + \mu_c - E_{pristine} + q\varepsilon_{VBM}$$

- ***CHARGED :*** ***the charged system calculation***
- ***Check.bash*** ***: a bash script to check the final calculations***
- ***FNV :*** ***the Freysoldt energy correction***
- ***NEUTRAL :*** ***the neutral defect system calculation (for reference only)***
- ***PRISTINE :*** ***the pristine system (formation energy + reference)***
- ***No_damp:*** ***SCPC-1 method without damp***
- ***SCPC-1 :*** ***the SCPC method using the neutral defect as reference***
- ***SCPC-2 :*** ***the SCPC method using the pristine system as reference***

Run the default VASP for the folders

CHARGED : ***the charged system calculation***

NEUTRAL : ***the neutral defect system calculation (for reference only)***

PRISTINE : ***the pristine system (formation energy + reference)***

No Damping SCPC-1 (neutral system as reference)

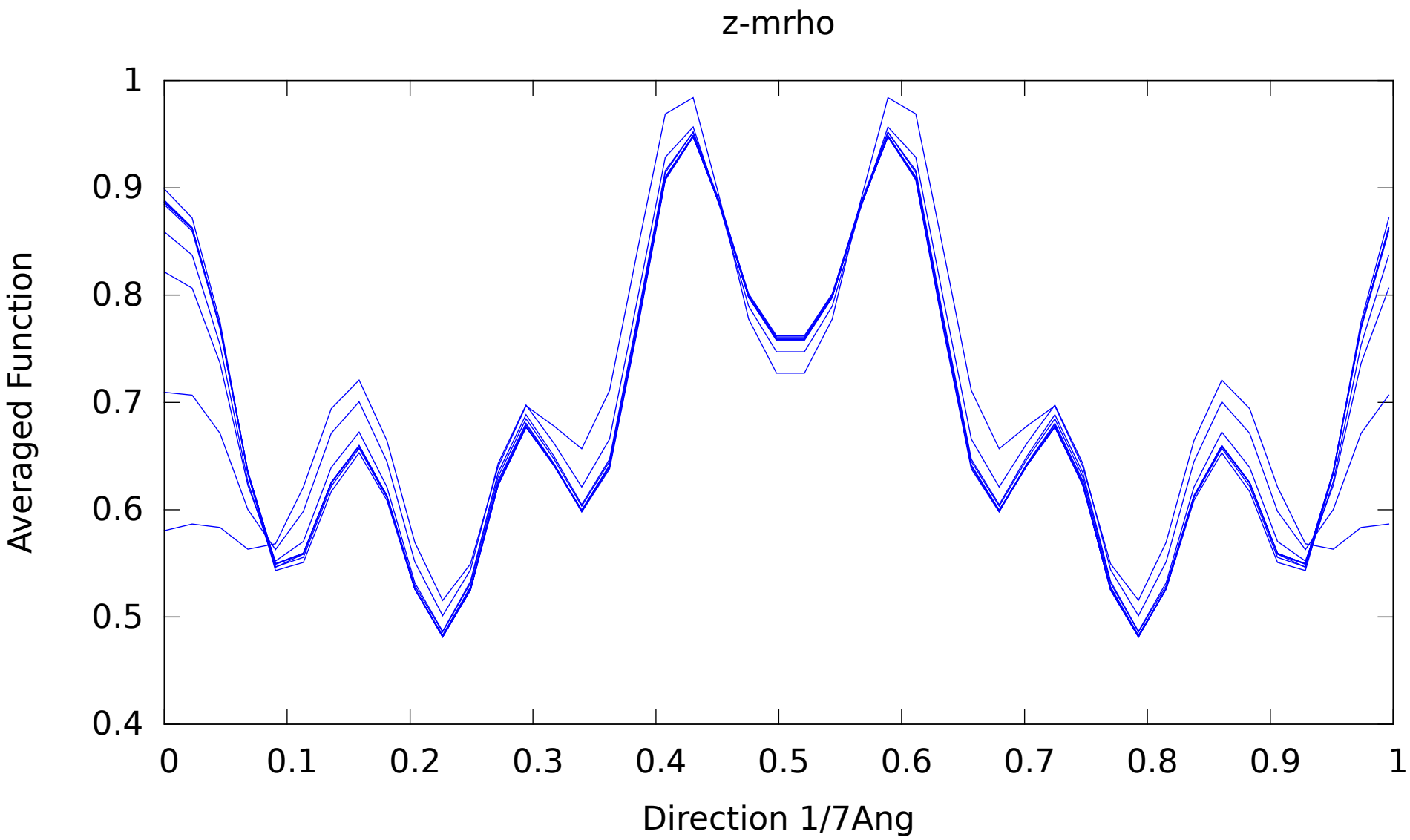
- ***From NEUTRAL:*** copy the CHGCAR to REFCHG and LOCPOT to REFPOT files into the SCPC-1 folder
- ***From the converged CHARGED:*** copy the CHGCAR to CHGCAR and the WAVECAR to WAVECAR into the SCPC-1 folder
- ***Inside the no_damp folder:***

INCAR	**CHGCAR → from charged calc.**
KPOINTS	**WAVECAR → from charged calc.**
POSCAR	**REFCHG → from neutral CHGCAR**
POTCAR	**REFPOT → from neutral LOCPOT**

INCAR without damped model

```
# Initial Guess
  ISTART = 1 ;
  ICHARG = 1 ;
#
  LWAVE  = F ;
  LCHARG = F ;
#
  NPAR = 2 ;
  NELECT = 254.0 ;
# Functional Definition
  GGA = PE ;
  LREAL = Auto ;
# Ionic Relax.
  IBRION = -1 ;
  ISIF   =  0 ;
  NSW    =  0 ;
#SCPC ;
  DOVCOR  =  T ;
  INVCOR  =  1 ;
  VCQTOT  = -2.00 ; formal charge
  VCDIEL  =  5.85 ; dielectric
#
```

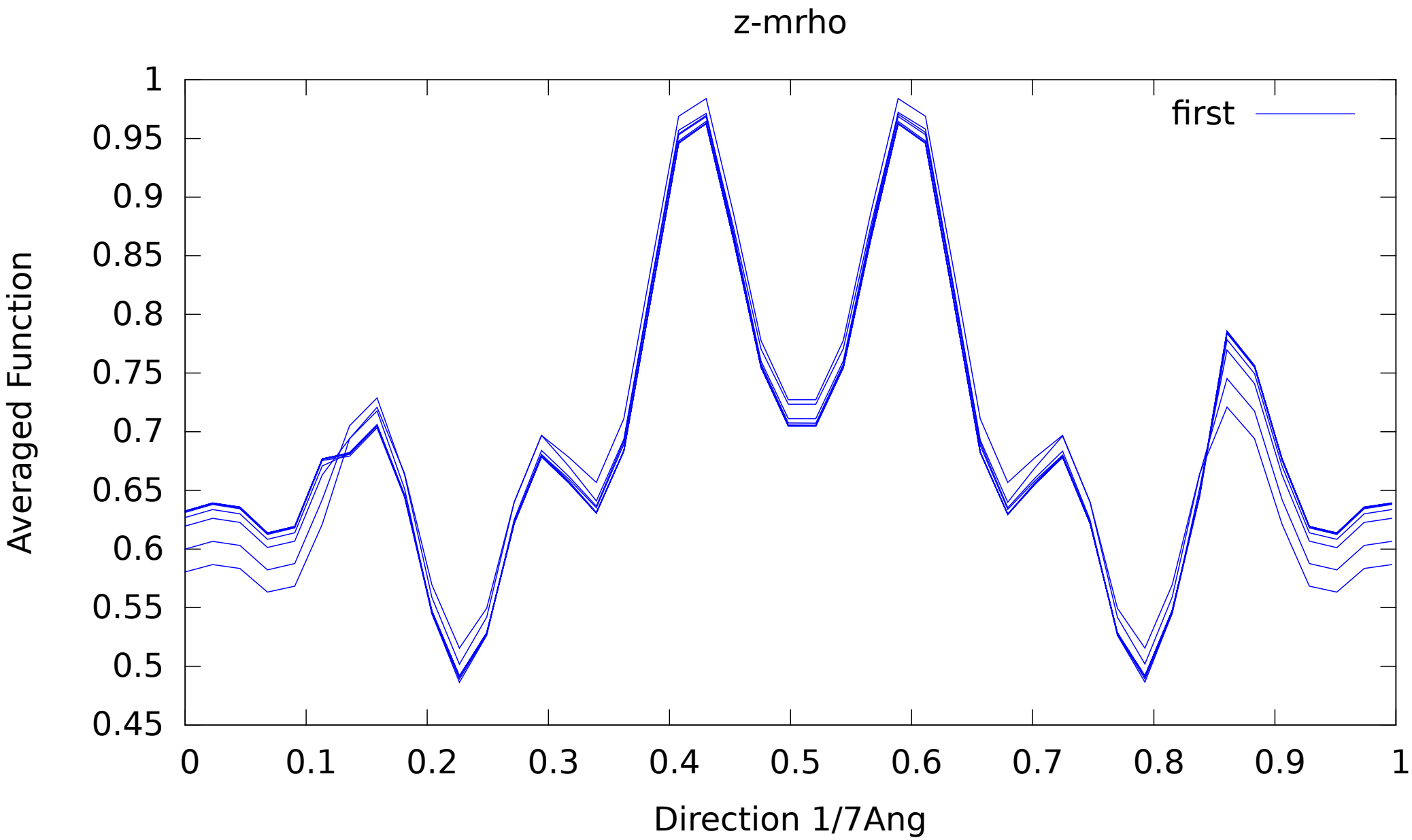
- There is not interface or broadening keywords!!!

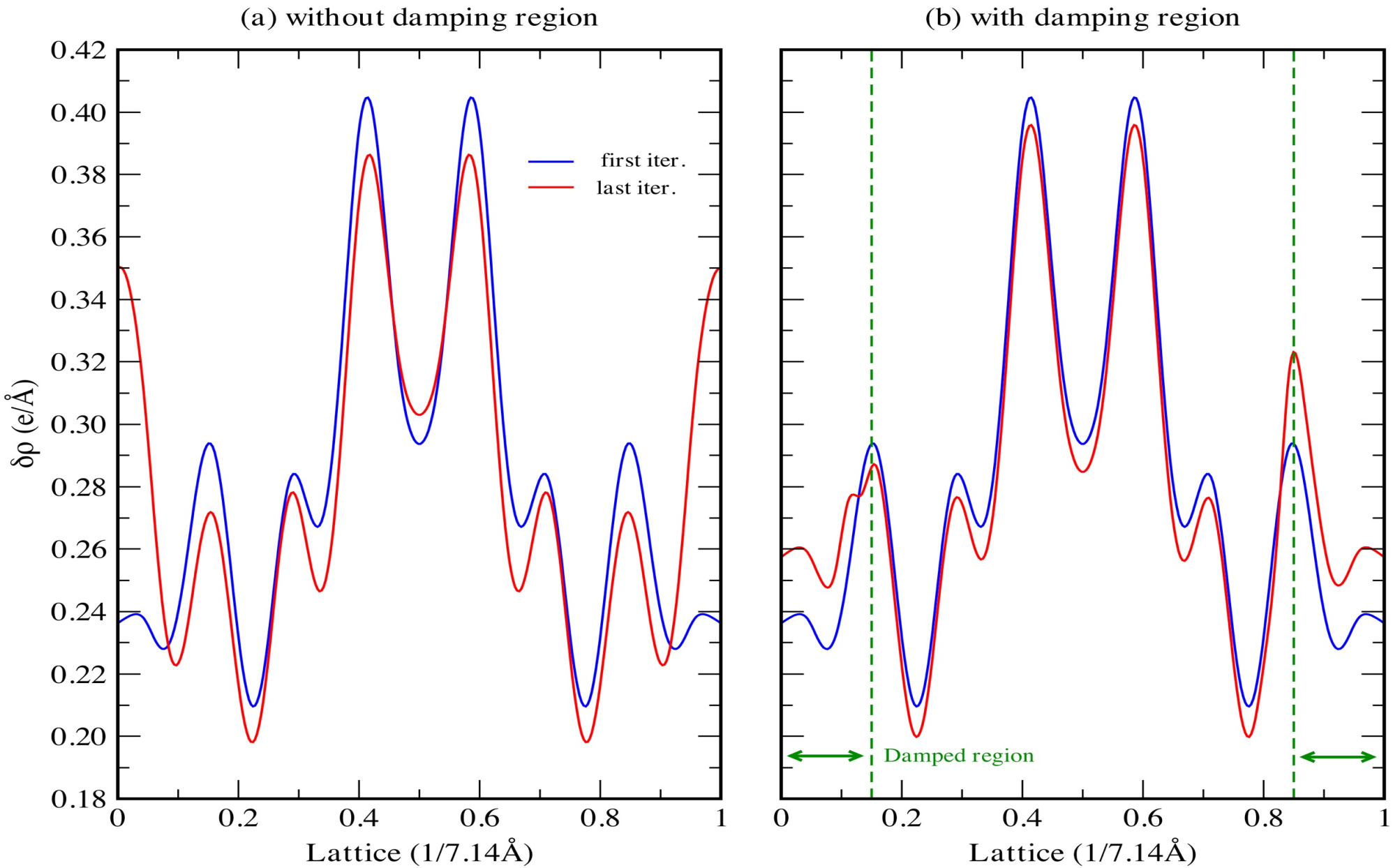

z-mrho
Averaged Function
Direction 1/7Ang
1
0.9
0.8
0.7
0.6
0.5
0.4
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

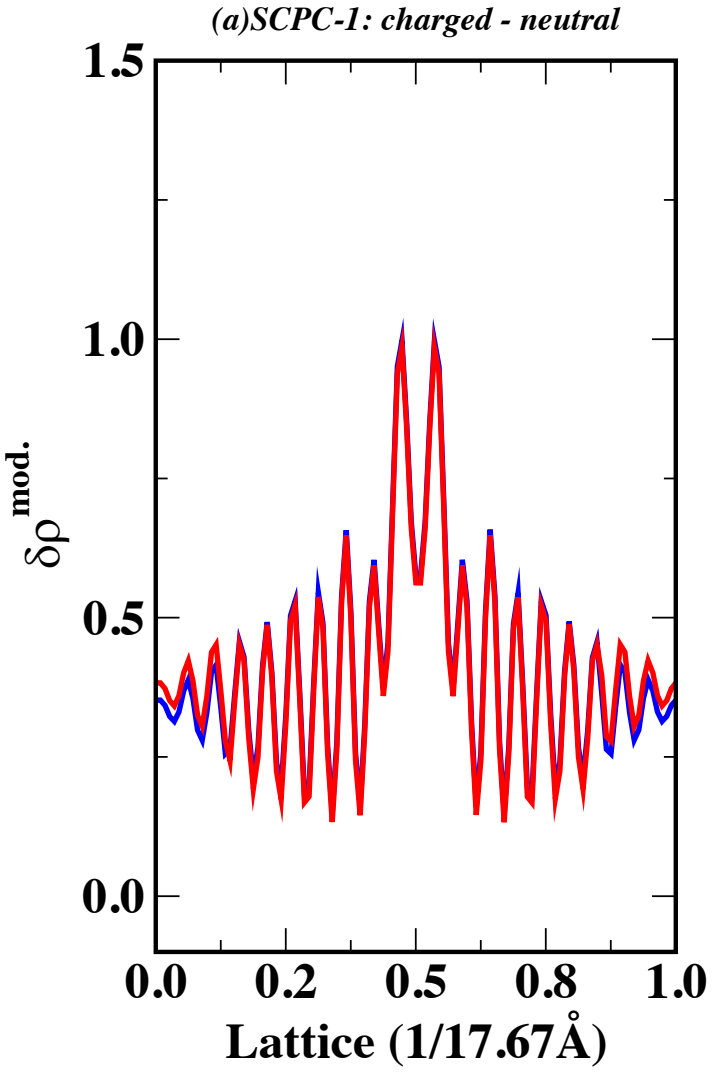
SCPC-1 (neutral system as reference)

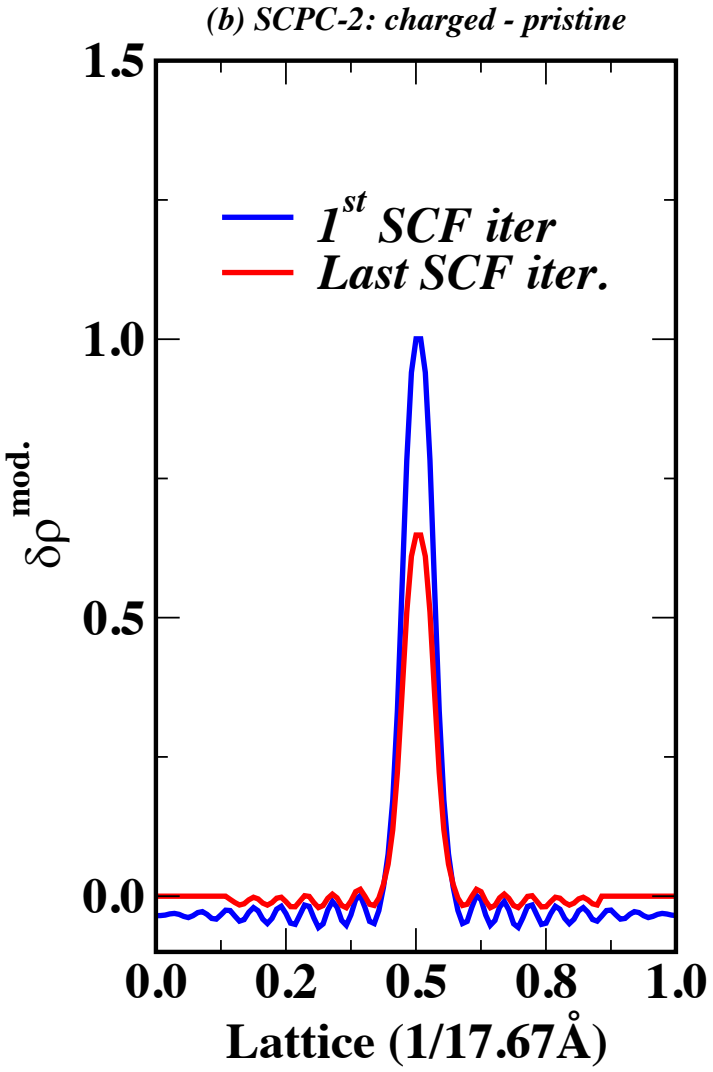
- ***From NEUTRAL:*** copy the CHGCAR to REFCHG and LOCPOT to REFPOT files into the SCPC-1 folder
- ***From the converged CHARGED:*** copy the CHGCAR to CHGCAR and the WAVECAR to WAVECAR into the SCPC-1 folder
- ***Inside the SCPC-1 folder:***

INCAR	**CHGCAR → from charged calc.**
KPOINTS	**WAVECAR → from charged calc.**
POSCAR	**REFCHG → from neutral CHGCAR**
POTCAR	**REFPOT → from neutral LOCPOT**


z-mrho
first
Averaged Function
Direction 1/7Ang
1
0.95
0.9
0.85
0.8
0.75
0.7
0.65
0.6
0.55
0.5
0.45
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1


(a) without damping region
(b) with damping region
first iter.
last iter.
δρ (e/Å)
Lattice (1/7.14Å)
Lattice (1/7.14Å)
Damped region
0.42
0.40
0.38
0.36
0.34
0.32
0.30
0.28
0.26
0.24
0.22
0.20
0.18
0
0.2
0.4
0.6
0.8
1





- For larger unit cells the damping is not so necessary due to the screening charge decay with the unit cell length

Check Results

```
**** Reference System set to NEUTRAL DEFECT ****

 <<<< VC(2-) Formation Energy (eV) >>>>

 Plain Calculation           :  10.54
 Energy Correc. (FNV Method) :  12.92
 Self-cons. Pot Correc.      :  11.90


**** Reference System set to PRISTINE ****

 <<<< VC(2-) Formation Energy (eV) >>>>

 Plain Calculation           :  10.54
 Energy Correc. (FNV Method) :  12.92
 Self-cons. Pot Correc.      :  12.55
```