Self-consistent Potential Correction (SCPC) at VASP

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Overview

- Keywords description
- VCl(+) formation energy – slab model
- VC(2-) formation energy – bulk model
- O2.TiO2 abnormal Rydberg states
- VcNc(-) band structure

First Step

- Download the vasp-tutorial.tgz

%cp -r /scratch/mcsilva/vasp-scpc-tutorial.tgz ./
%tar zxvf vasp-scpc-tutorial.tgz
%cd vasp-scpc-tutorial
%ls *

bulk-diamond nv-bands o2tio2 nvcl-nacl-slab

SCPC Keywords

```
# SCPC
   DOVCOR   =  T       ;    T = true or F = false
   INVCOR    =  6      ;    which SCF step to start
   VCQTOT   = -1.00    ;    the defect charge
   VCZLOW   =  0.15    ;    lower interface  fractional coord.
   VCZHIG    =  0.34   ;    higher interface fractional coord.
   VCDIEL    =  6.68   ;    macroscopic dielectric
   VCBROAD =  0.70     ;    broadening for the boxcar function
   VCPRTX    =  T      ;    printing the averages in X direction
   VCPRTY    =  T      ;    printing the averages in Y direction
   VCPRTZ    =  T      ;    printing the averages in Z direction
   VCRXCUT  =  0.15    ;    damping region in X direction frac. coord
   VCRYCUT  =  0.15    ;    damping region in Y direction
   VCRZCUT  =  0.15    ;    damping region in Z direction
#
```

Dielectric

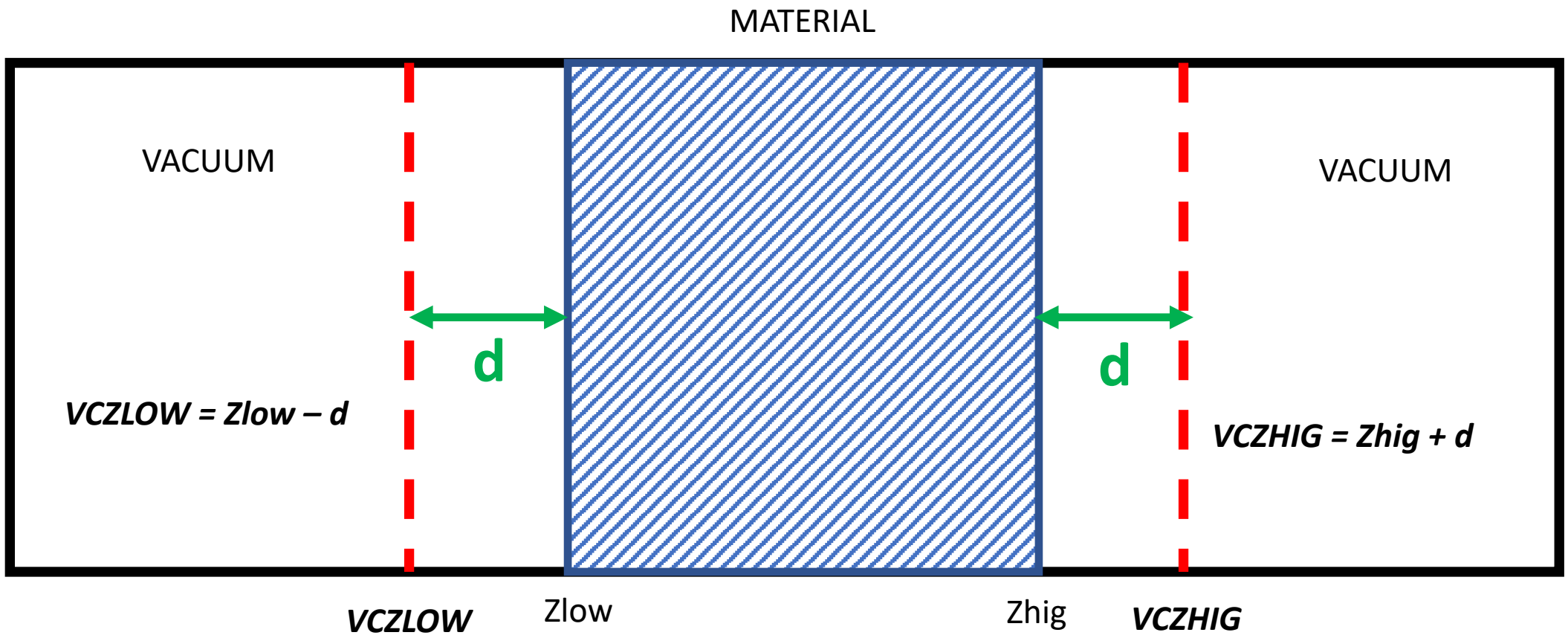
```
# SCPC
     VCDIEL     =  6.68    ;     macroscopic dielectric
#
```

$$\begin{pmatrix} \varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\ \varepsilon_{yx} & \varepsilon_{yy} & \varepsilon_{yz} \\ \varepsilon_{zx} & \varepsilon_{zy} & \varepsilon_{zz} \end{pmatrix} \Rightarrow \begin{pmatrix} \varepsilon_{xx} & 0 & 0 \\ 0 & \varepsilon_{yy} & 0 \\ 0 & 0 & \varepsilon_{zz} \end{pmatrix}$$

$$\text{VCDIEL} = \begin{cases} \dfrac{\left(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}\right)}{3} \\ \left(\varepsilon_{xx} * \varepsilon_{yy} * \varepsilon_{zz}\right)^{1/3} \end{cases}$$

Interface

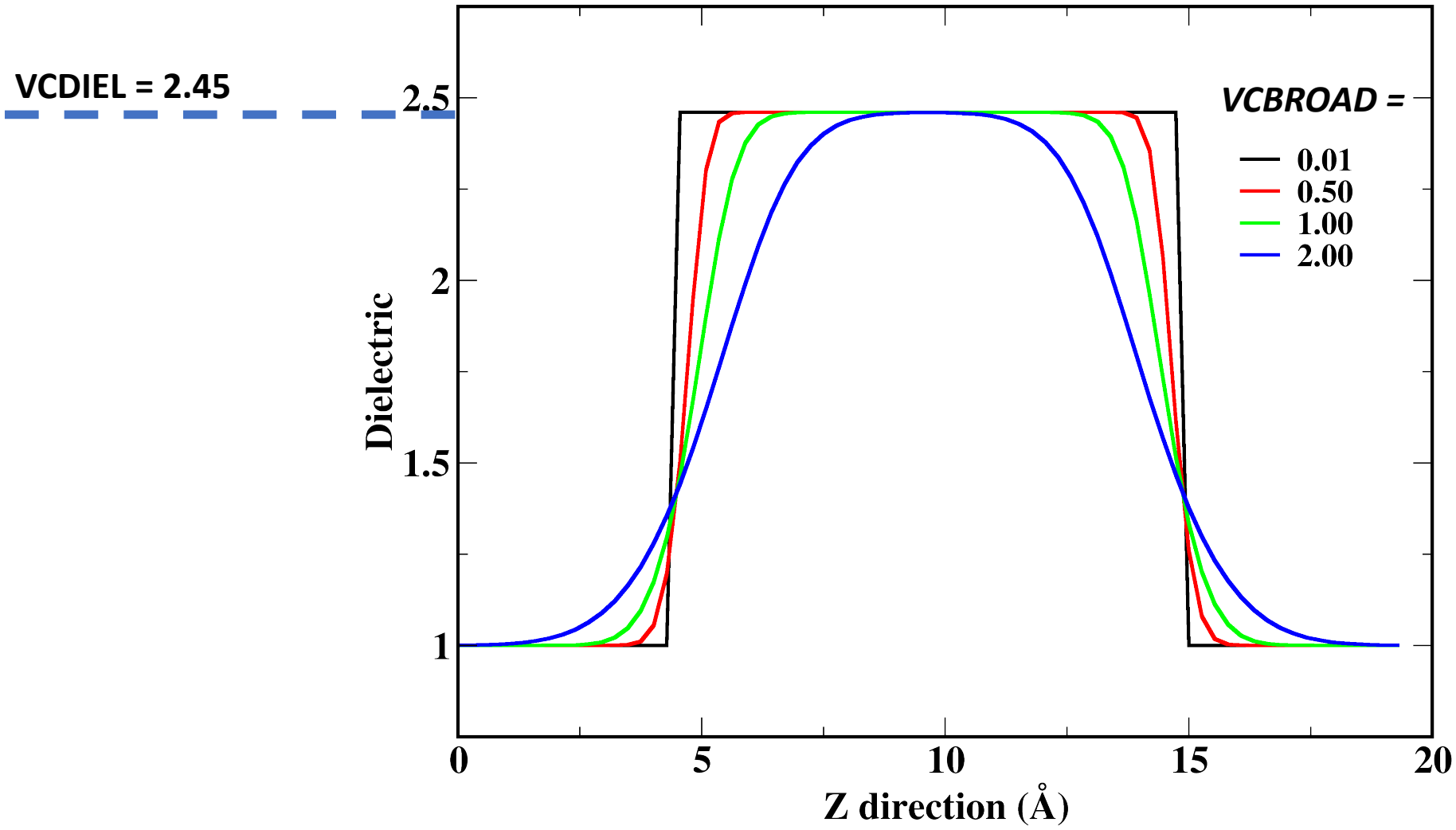
```
# SCPC
   VCZLOW   =  0.15   ;    lower interface coord.
   VCZHIG   =  0.34   ;    higher interface coord.
#
```



- **d** symmetric
- **d** ≈ 1.0 – 2.0 Å

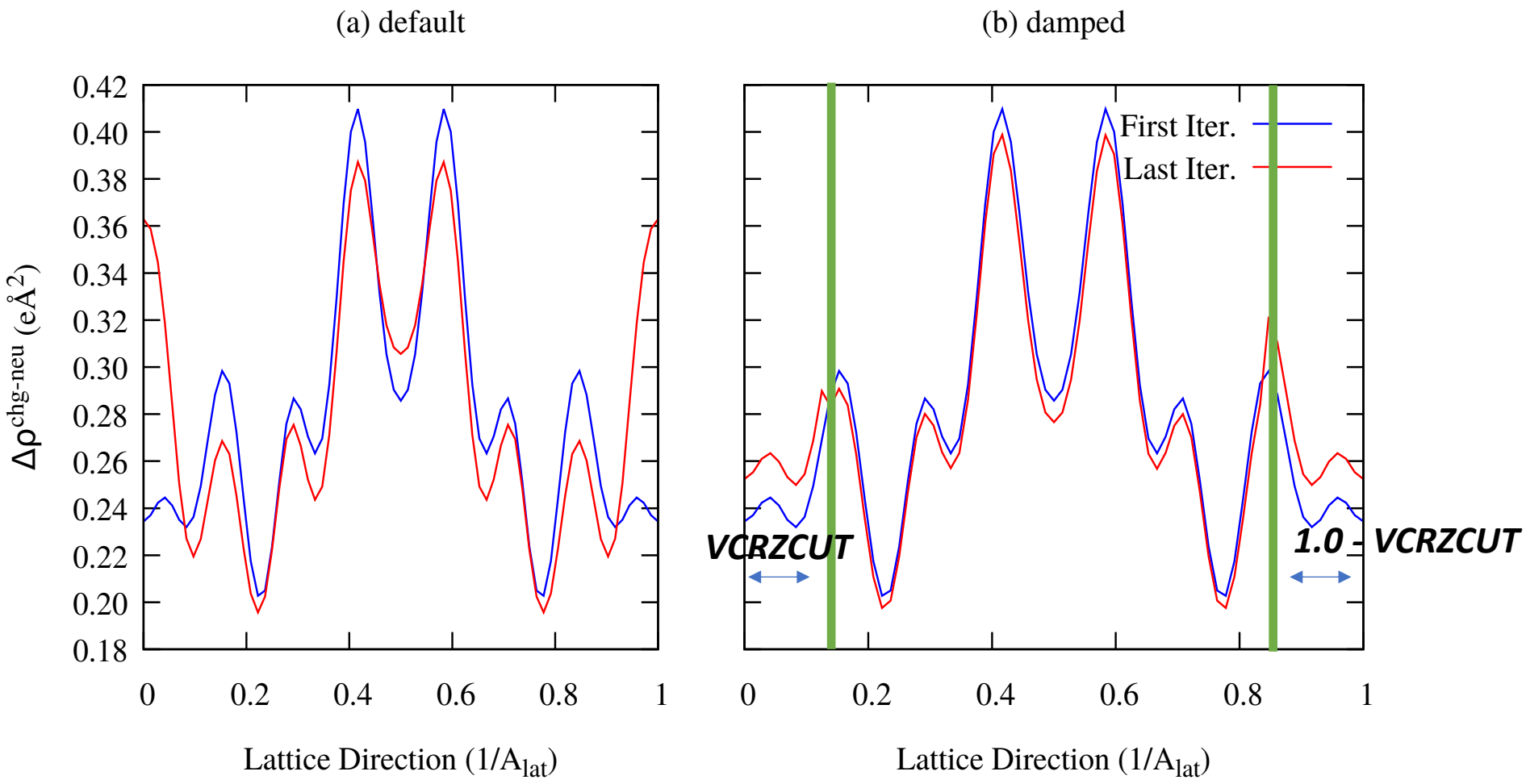
Broadening

```
# SCPC
   VCBROAD =  0.70   ;     broadening for the boxcar function
#
```

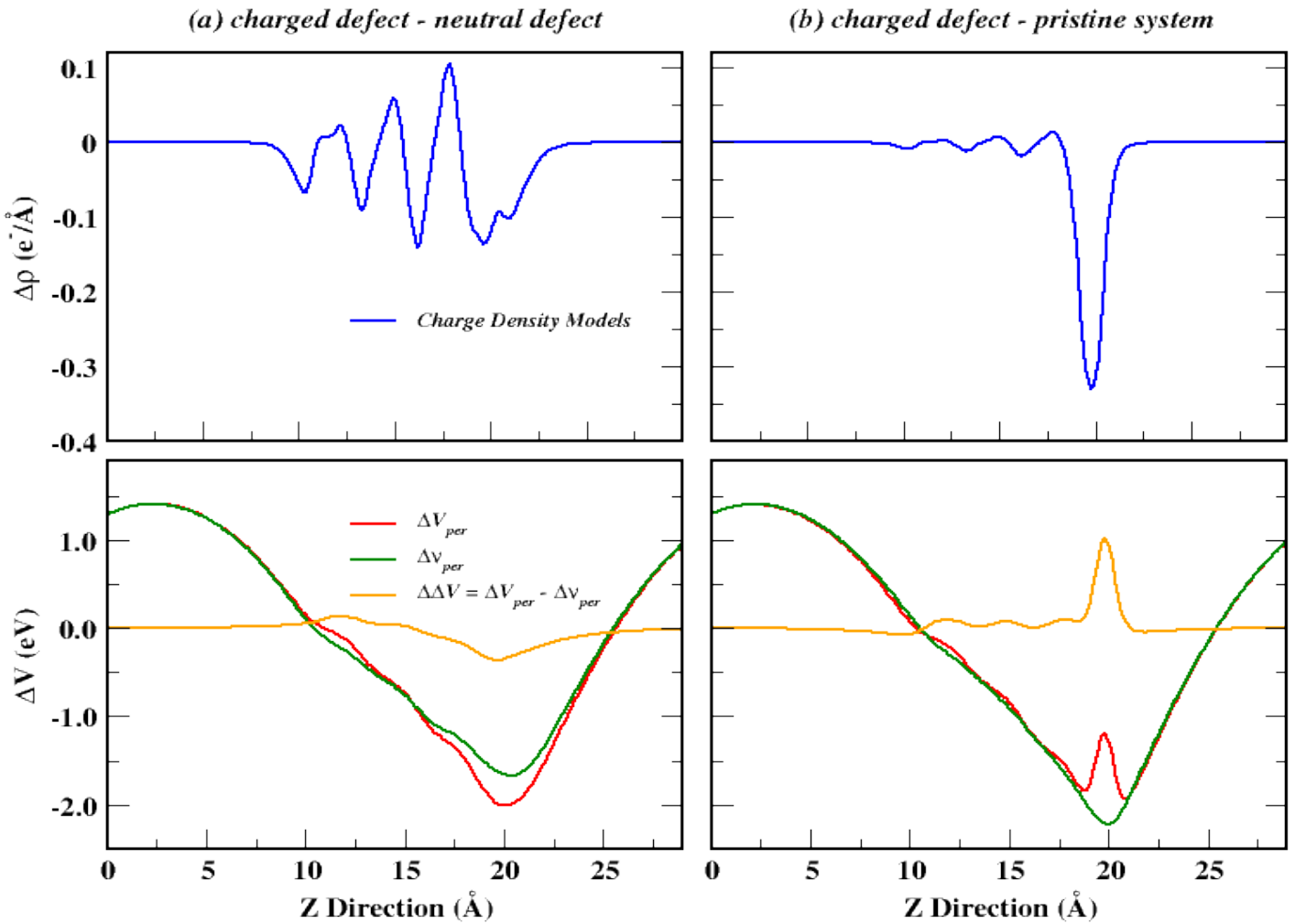


Damping Effect

```
# SCPC
   VCRXCUT  =  0.15   ;    damping region in X direction
   VCRYCUT  =  0.15   ;    damping region in Y direction
   VCRZCUT  =  0.15   ;    damping region in Z direction
#
```



Charge and Potential Model



- To be controlled by external file

REFCHG: reference CHGCAR
REFPOT: reference LOCPOT

Outputs

CHG	INCAR	MGSolver_PER103	REFCHG	VCOROUT	
CHGCAR	KPOINTS	MGSolver_PER105	REFPOT	WAVECAR	
CONTCAR	LinkRefFiles.bash	OSZICAR	REPORT	XDATCAR	
CopyInitFiles.bash	MGSolver_COR102	OUTCAR	scpc-1.log	z-diel.dat	
DOSCAR	MGSolver_COR104	PCDAT	scpc-1.pbs	z-mpot.dat	
EIGENVAL	MGSolver_COR106	POSCAR	vasp.out	z-mrho.dat	
IBZKPT	MGSolver_PER101	POTCAR	vasprun.xml	z-vcor.dat	

REFCHG and REFPOT: these are the reference charge and potential system.

VCOROUT: this file contains important information about the method and the **Potential Alignment**.

MGSolver_*: these are from the Poisson Solver function, you can remove in the end

z-*.dat: these are debug files for the averages, you can remove in the end

vasp.out

```
# SCPC
  INVCOR    = 4 ;
#
```

entering main loop

	N	E	dE	d eps	ncg	rms	rms(c)
DAV:	1	0.122203658387E+04	0.12220E+04	-0.46363E+04	824	0.375E+02	
DAV:	2	-0.166489834304E+02	-0.12387E+04	-0.11937E+04	988	0.151E+02	
DAV:	3	-0.193739329501E+03	-0.17709E+03	-0.17587E+03	952	0.628E+01	
DAV:	4	-0.198328856695E+03	-0.45895E+01	-0.45809E+01	920	0.125E+01	
DAV:	5	-0.198455967031E+03	-0.12711E+00	-0.12701E+00	952	0.190E+00	BRMIX: very serious problems

This is not SCF cycles, it is the NSCF Harris functional to the initial guess

the old and the new charge density differ

old charge density: 249.00000 new 247.99972

0.169E+02

DAV:	6	-0.122064155629E+03	0.76392E+02	-0.12143E+02	780	0.155E+01	0.109E+02	*The SCF starts here*
DAV:	7	-0.779308467966E+02	0.44133E+02	-0.50470E+01	928	0.109E+01	0.151E+01	
DAV:	8	-0.129811071850E+03	-0.51880E+02	-0.20340E+01	872	0.714E+00	0.106E+01	
DAV:	9	-0.151324946680E+03	-0.21514E+02	-0.78074E+00	904	0.392E+00	0.808E+00	

<<< Self-consitent Potential Correction is ON >>>

INVCOR = 4 ;

DAV:	10	-0.169686791997E+03	-0.18362E+02	-0.81729E+00	896	0.439E+00	0.690E+00

VCOROUT

<<<< SELF-CONSISTENT POTENTIAL CORRECTION - SCPC >>>>

SCPC will start at cycle : 6

Total model charge: 1.0

Interface coord. low bound: 0.23
Interface cood. high bound: 0.76
Interface broadening: 0.40
Interface avg. dielectric: 2.46

Cell volume: 0.2441041756E+04
Cell lattice: 11.173000 11.173000 19.554000

Model grid: 45 45 73
Model step size grid: 0.248289 0.248289 0.267863

VCOROUT

Integrated Reference RHO: 0.2489997194E+03 249 elec.
Integrated Reference VHAR: 0.8890971147E-11 Must be close to ZERO

<<<< SCPC Cycle: 6 >>>>

Integrated System RHO : 0.2479997208E+03 248 elec.
Integrated System VHAR : -0.2096587115E-10 Must be close to ZERO

Positive defect

Mixing RHO: 1.0000 Ignore this, I have to remove it from here

Mixing RXCUT: -1.0000
Mixing RYCUT: -1.0000 Damping region (-1.0 to turn off)
Mixing RZCUT: -1.0000

Energy Correction : 0.2900 eV
Potential Alignment (X,Y,Z): 0.075440 0.075440 0.075440 eV

This is important for formation energy calculation