VASP Notes….

**1. Define k-points**

**INCAR**

ENCUT = 400

EDIFF = 1E-5

NWRITE = 2

PREC = Accurate

ISMEAR = -5

**Script: mallak.exe**

#!/bin/bash

rm -f WAVECAR

for i in 4 6 8 10 12 14 16 18 20 22 24 26

do

cat > KPOINTS.$i << FIN

#malla de $i $i $i

0

G

$i $i $i

0 0 0

FIN

cp KPOINTS.$i KPOINTS

echo "\*\*\* corriendo $i"

mpirun -np 4 vasp

cp OUTCAR OUTCAR.$i

echo "\*\*\*termino $i"

echo

done

**2. Fix k-points and define ENCUT**

**Script: ENCUT.exe**

#!/bin/bash

rm -f WAVECAR

for i in 320 360 400 440 480 500 520 540 560 600

do

cat > INCAR.$i << FIN

ENCUT=$i

EDIFF=1E-05

NWRITE=2

PREC=Accurate

ISMEAR=-5

FIN

cp INCAR.$i INCAR

echo "\*\*\* corriendo $i"

mpirun -np 4 vasp

cp OUTCAR OUTCAR.$i

echo "\*\*\* termino $i"

echo

done

**3. Relax your structure**

**INCAR**

SYSTEM = AlAs(8atomos)

NWRITE = 3

PREC = Accurate

ADDGRID = .TRUE.

ISMEAR = -5

ISTART = 0

LAECHG = .TRUE.

LWAVE = .TRUE.

ENCUT = 520.0

EDIFF = 1E-06

LREAL = .FALSE.

NELMIN = 6

EDIFFG = 1E-05

NSW = 60

IBRION = 2

ISIF = 3

ISYM = 2

**4. Self-consistency (SCF)**

**INCAR**

SYSTEM = AlAs(64 atomos)

IBRION = -1

ISTART = 0

ISMEAR = -5

ENCUT = 520.0

EDIFF = 1E-06

NELMIN = 6

NCORE = 4

LREAL = Auto

ISPIN = 2

MAGMOM = 30\*0.7 32\*0.7 2\*0.7

**5. Density of states (duplicate k-points and run it in the same file as SCF)**

**INCAR**

SYSTEM = AlAs(64 atomos)

ICHARG = 11

ISMEAR = -5

ENCUT = 520.0

LORBIT = 11

NEDOS = 3000

NELMIN = 6

NCORE = 4

LREAL = Auto

ISPIN = 2

MAGMOM = 30\*0.7 32\*0.7 2\*0.7

**6. Bands (change k-points for high symmetry paths and run it in the same file as SCF)**

**INCAR**

SYSTEM = AlAs

ICHARG = 11

ISMEAR = 0

SIGMA = 0.1

ENCUT = 520.0

LORBIT = 11

NELMIN = 6

NCORE = 4

LREAL = Auto

ISPIN = 2

MAGMOM = 30\*0.7 32\*0.7 2\*0.7