

# MASTANI 2014

## DAY 2 – exercise 3

scf and band structure calculations for Cu (metal)

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- No input files available, but should be generated for practice.
- Next two slides explain where changes need to be done for scf calculations.
- Follow the similar procedure to find dos and band structure for Cu.
- Refer to [http://www.quantum-espresso.org/wp-content/uploads/Doc/INPUT\\_PW.html](http://www.quantum-espresso.org/wp-content/uploads/Doc/INPUT_PW.html) for more details

```
&control  
  calculation = 'scf',  
  verbosity = 'high'  
  prefix = 'Al_exc2'  
  outdir = './tmp/'  
  pseudo_dir = '../pseudo/'  
/
```

```
&system  
 ibrav = 2,  
celldm(1) = 7.65,  
nat = 1,  
ntyp = 1,  
ecutwfc = 12.0,  
occupations = 'smearing',  
smearing = 'marzari-vanderbilt',  
degauss = 0.02  
/
```

```
&electrons  
  mixing_beta = 0.7  
/
```

```
ATOMIC_SPECIES  
Al 26.98 Al.pz-vbc.UPF
```

```
ATOMIC_POSITIONS (alat)  
Al 0.0 0.0 0.0
```

```
K_POINTS (automatic)  
6 6 6 1 1 1
```

- Not system dependent!
- “**prefix**” should be changed preferably to avoid overwriting of wavefunctions and charge density.

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Al 26.98 Al.pz-vbc.UPF

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```
K_POINTS (automatic)
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```

1. What is the **crystal structure** for Cu?

2. Cu experimental **lattice constant** as a starting point?

3. **Number of atoms** in the unit cell?

4. How many **different types of elements**?

Need to specify **which element**,  
**which pseudopotential**, and  
**atomic positions correct**?

Convergence tests required  
for the new pseudopotential!!

NOTE – Cu pseudopotential available in day2/pseudo directory