Karlsruhe Institute of Technology

The ABC of DFT: hands-on training AIMS 3

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INSTITUTE OF NANOTECHNOLOGY

Getting started

- The input files for and descriptions of the exercises are contained in a tar file `handsonsession.8.tar` under `/net/intact/home/dft20>`
- Please copy them to your account and unpack

```
> cp ~/../dft20/handsonsession.8.tar ~/ABC_of_DFT/hands-on-sessions/
> cd ~/ABC_of_DFT/hands-on-sessions
> tar -xvf handsonsession.8.tar
```

- If you did not do this last time:

```
> cp ~/../dft20/setupaims .
> ./setupaims
```

- For VESTA vesion 3:

```
> cp -r ../dft20/VESTA-i686/ ~/
```

- AIMS can now be executed by typing

```
> aims
```

Or better

```
> aims | tee outputfilename
```

Exercises

- Two dimensional systems

- Graphene:
  - One more parameter to converge
  - Band structure
  - Density of states
  - Workfunction

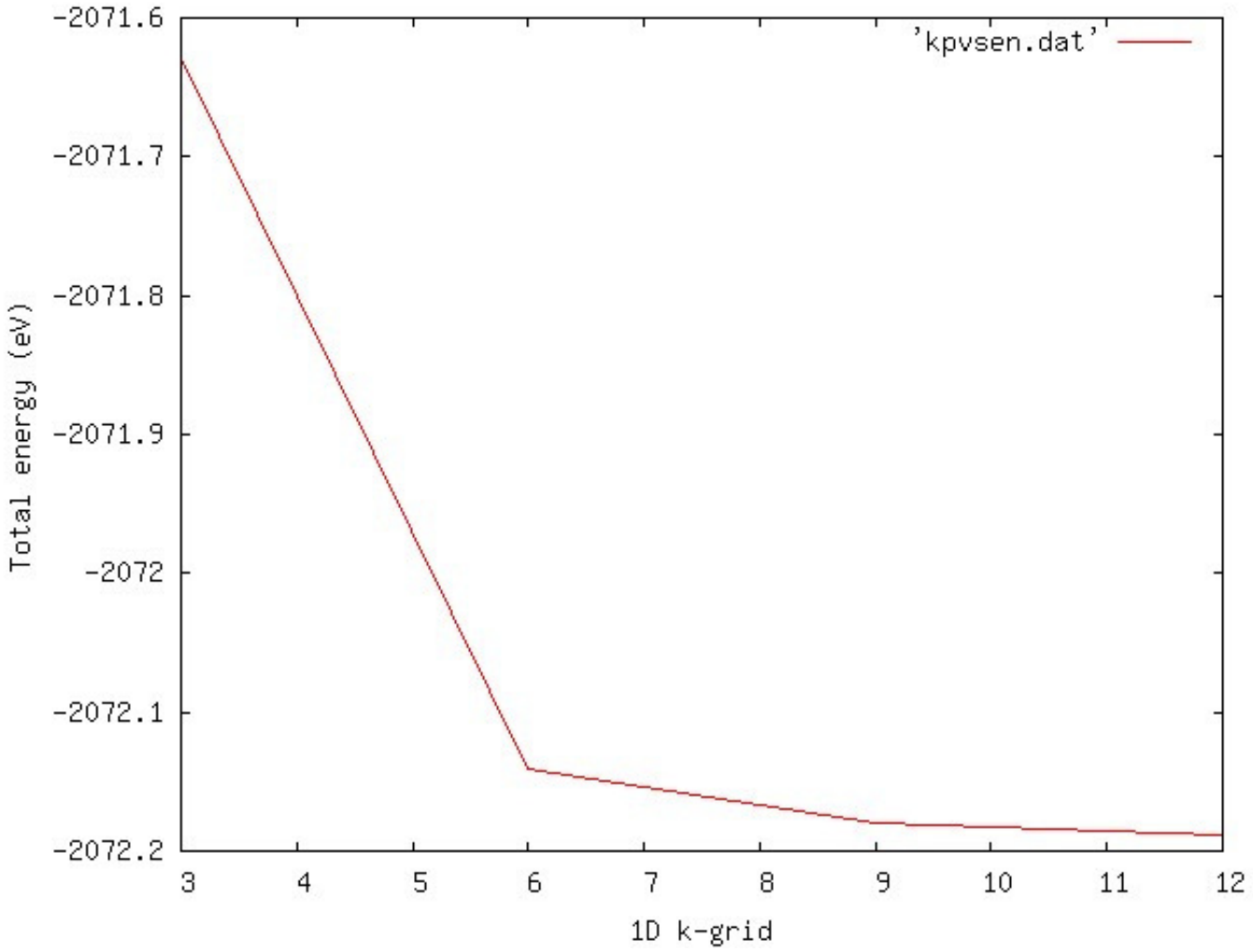
  - Defects: Super cells

- Layered materials

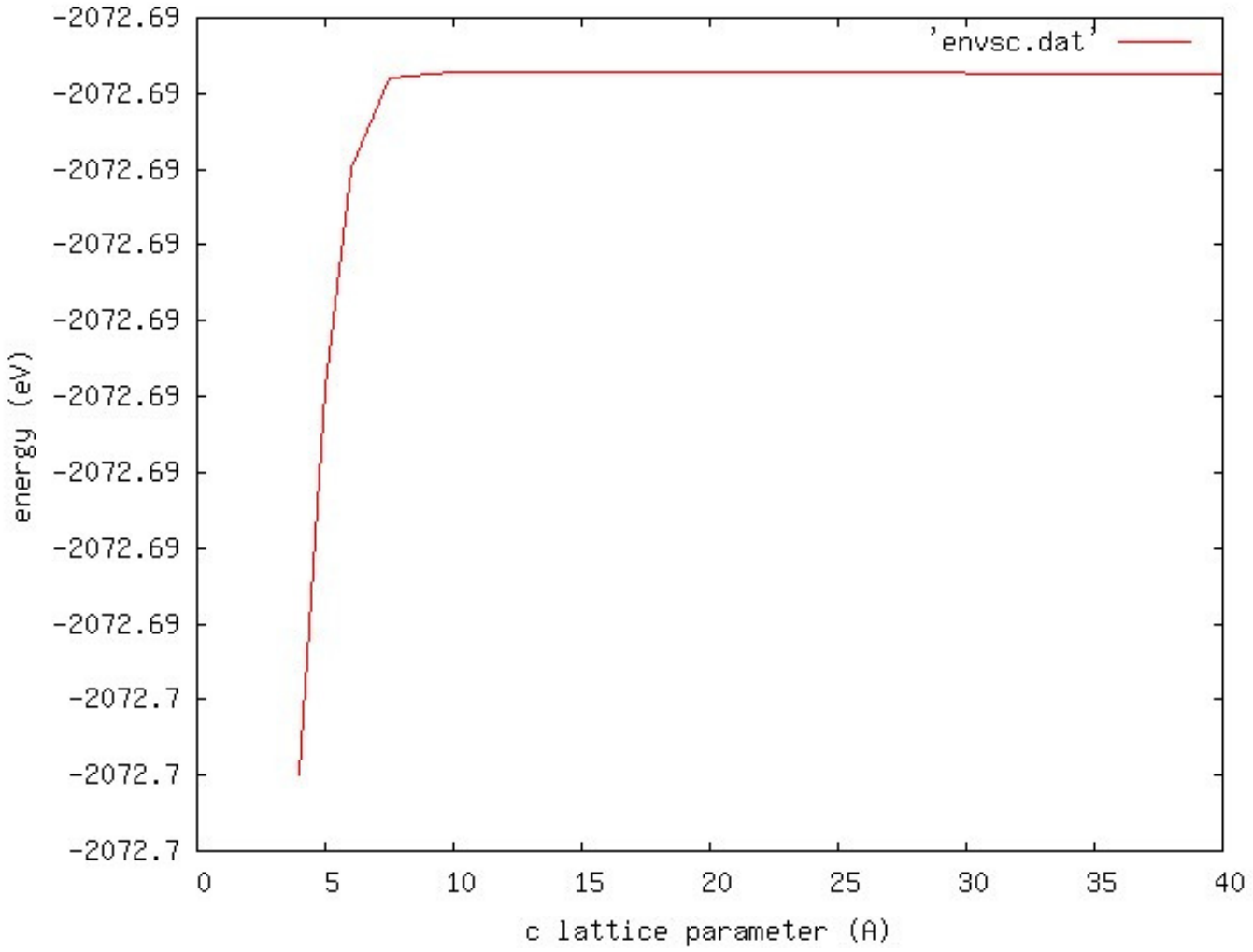
Check the convergence of the total energy

- What k-point grid would you use? (what series of grids would use checking convergence)
- And with respect to the c-lattice parameter
- Also look at the fermi energy as a function of c and the total time of the calculation
  - What do you notice?

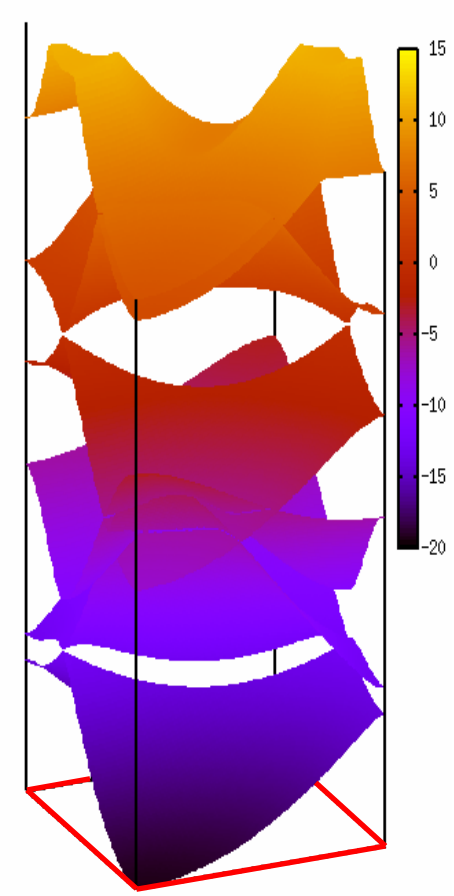
K-point convergence

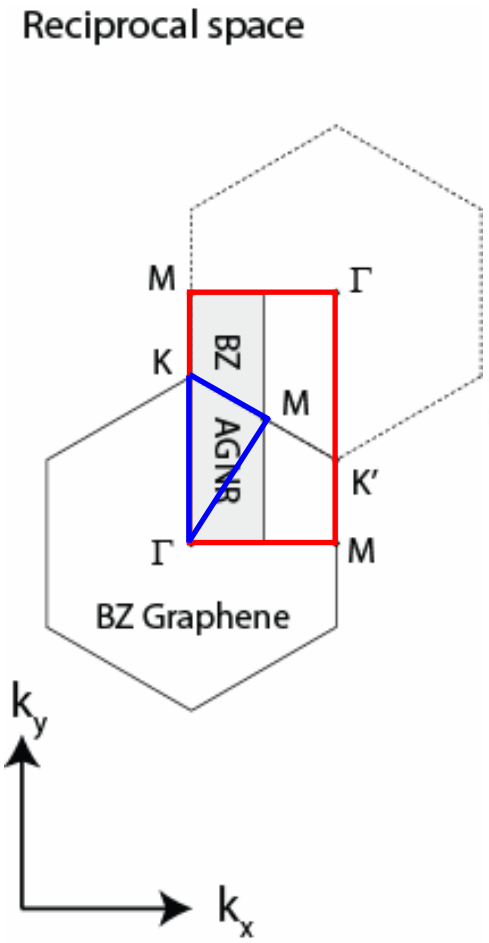


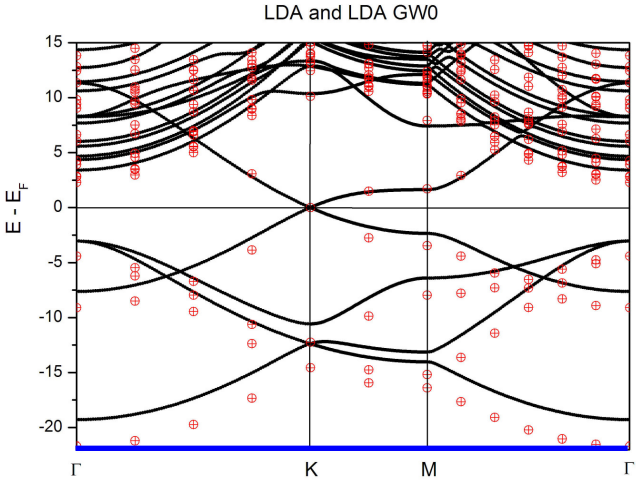
One more parameter to converge



Dispersion of graphene



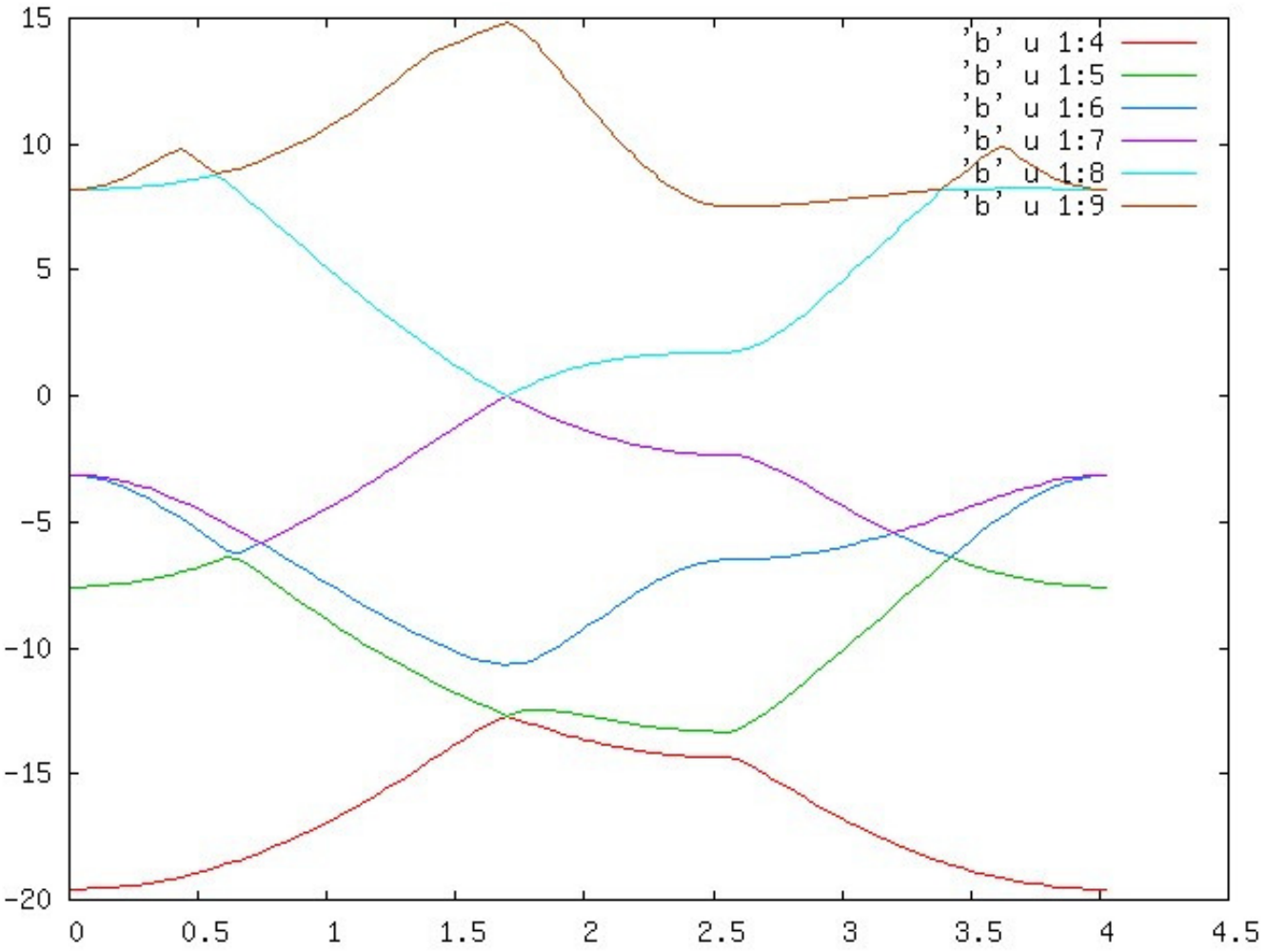




$\varepsilon_i(k_x,k_y)$

A. Dasgupta, S. Bera, F. Evers, M.J. van Setten, Phys. Rev. **85**, 125433 (2012)

Errors in plotting a bandstructure



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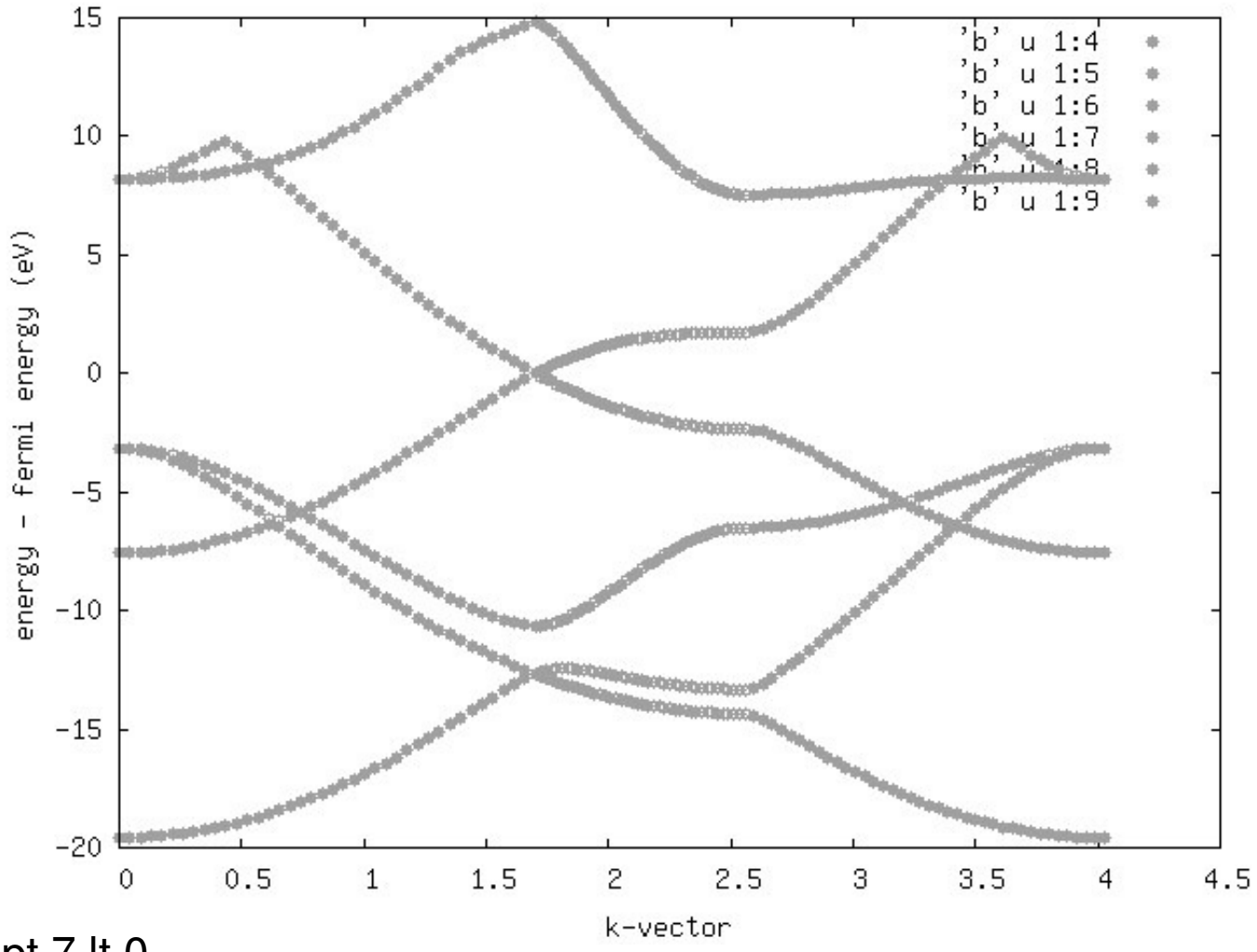
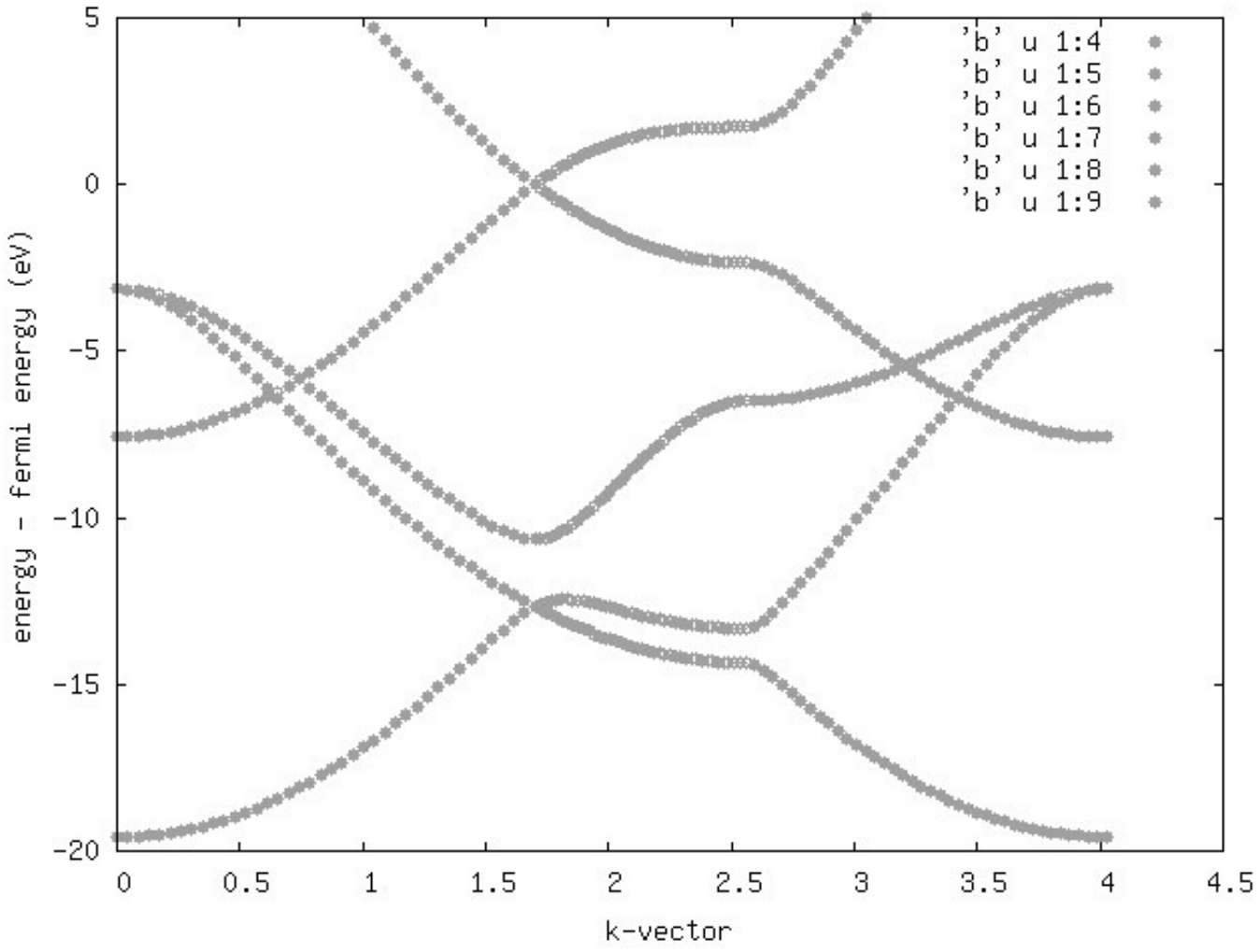
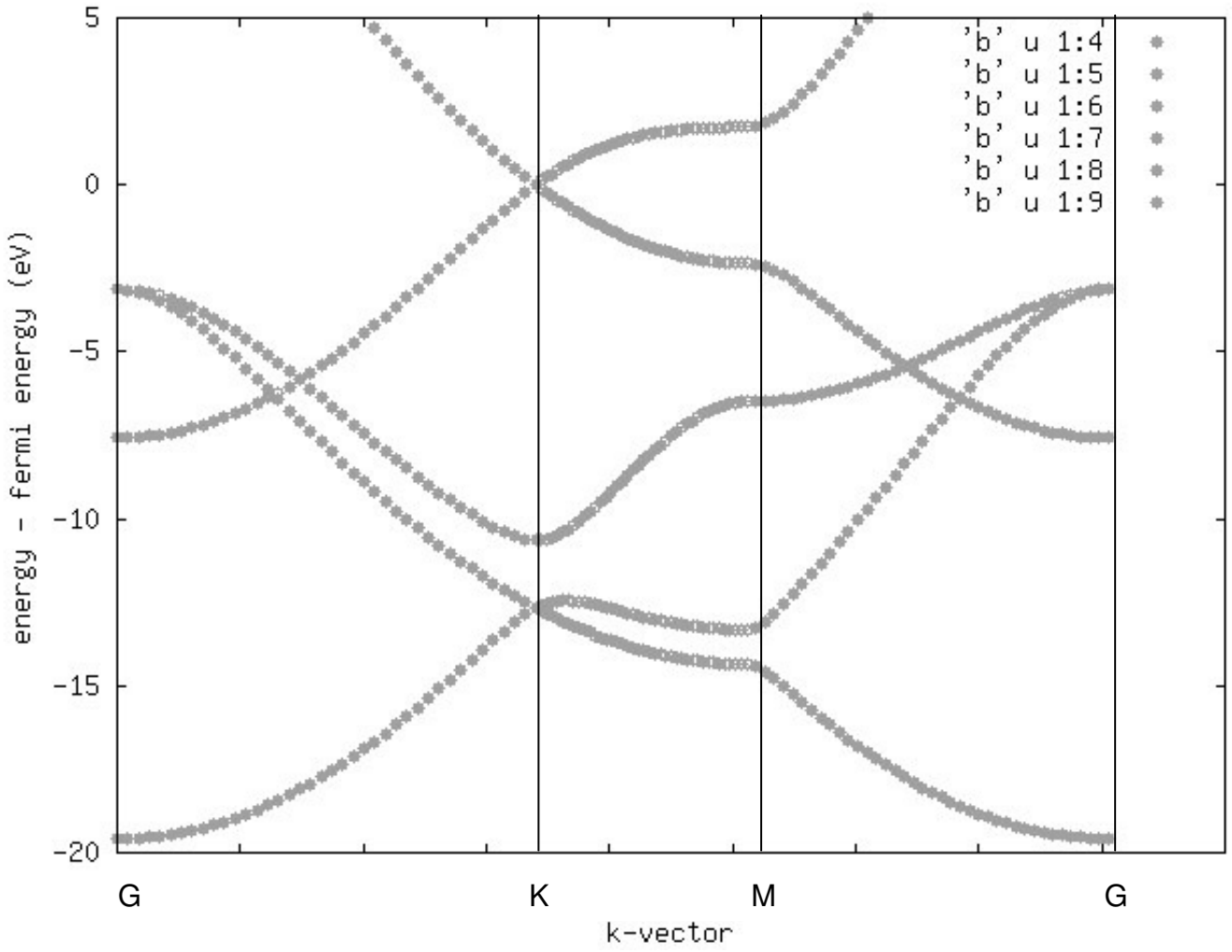


plot ‘’ w p pt 7 lt 0

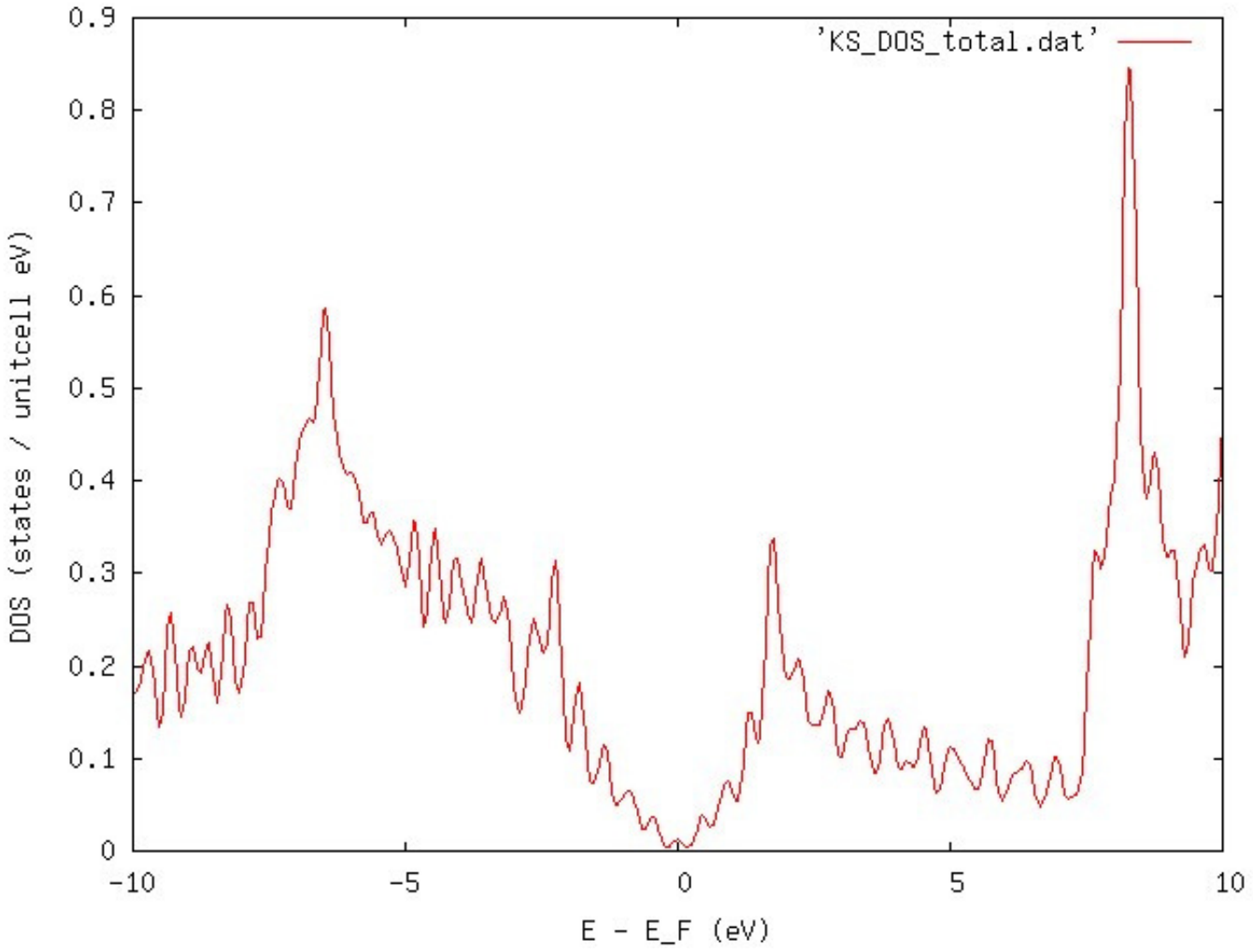
Errors in plotting a bandstructure



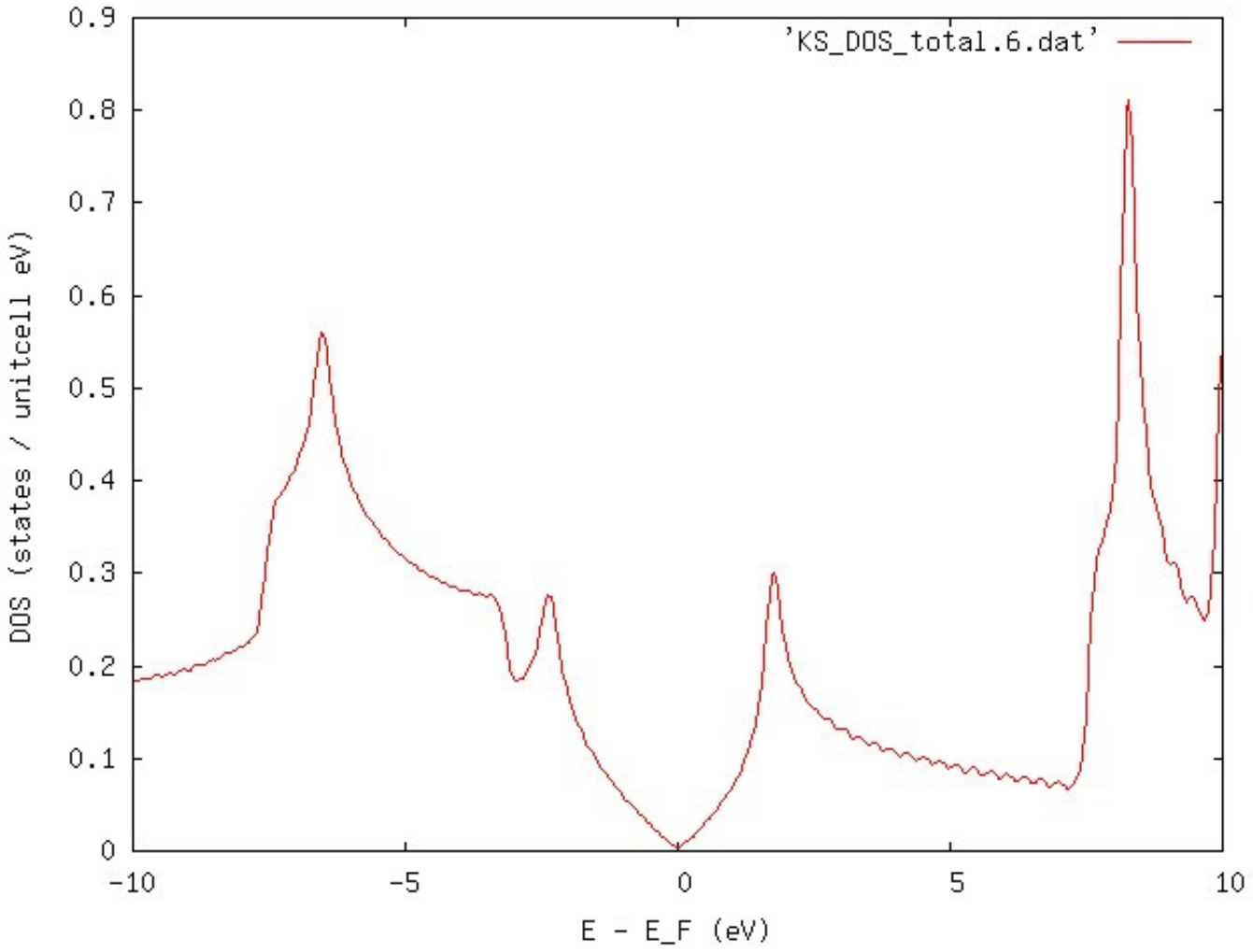
Correctly plotting a bandstructure



Density of states



Density of states



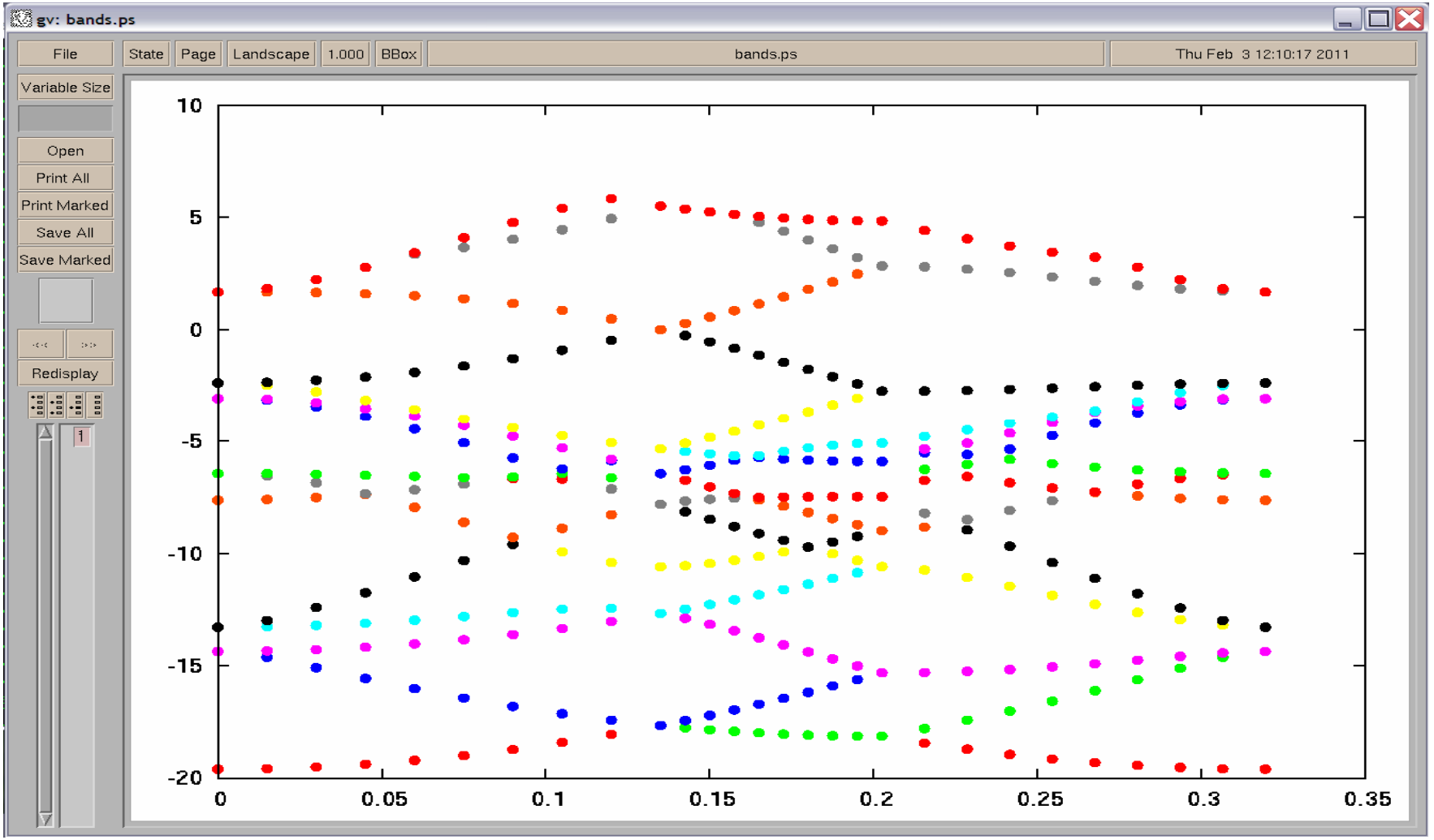
Workfunction

- The amount of energy to pay to remove one electron
- Why did the HOMO energy converge so badly?

Workfunction

- The amount of energy to pay to remove one electron
- Why did the Fermi energy converge so badly?
- Add a correction:
  - Uncomment `evaluate_work_function`
  - and `set_vacuum_level`

02 Bands 2 2 1 super cell



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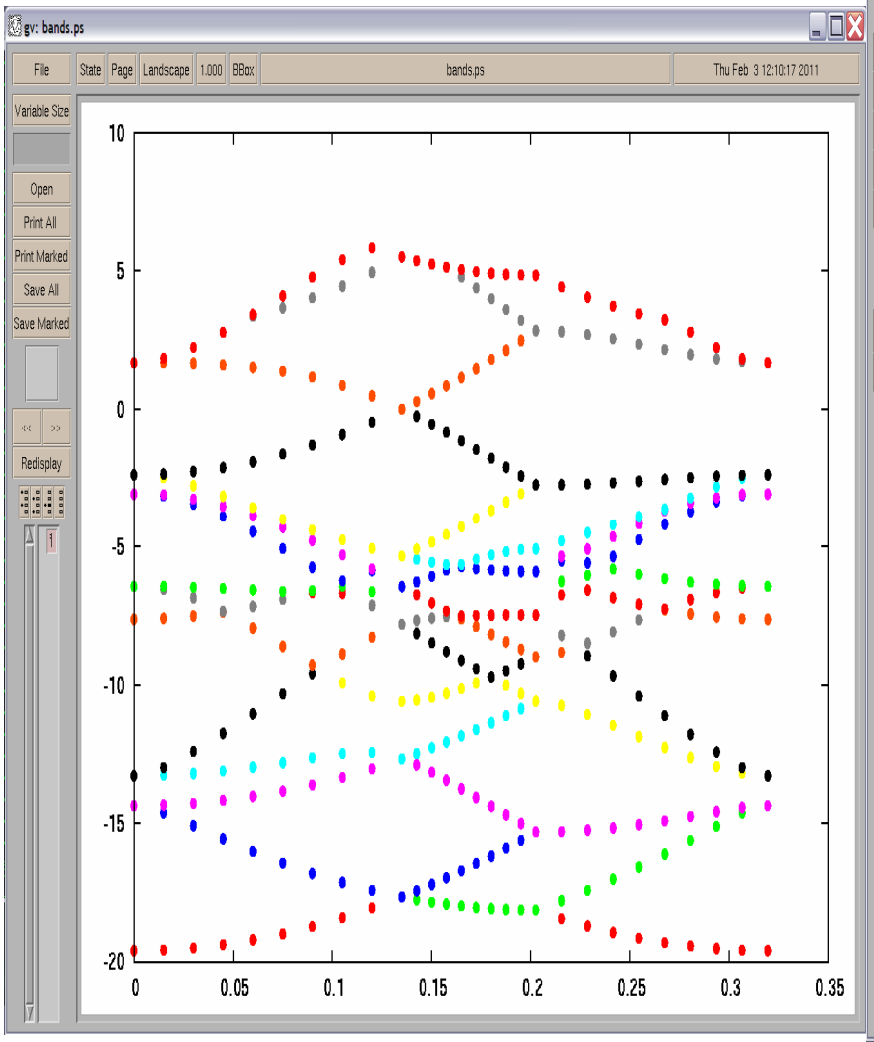
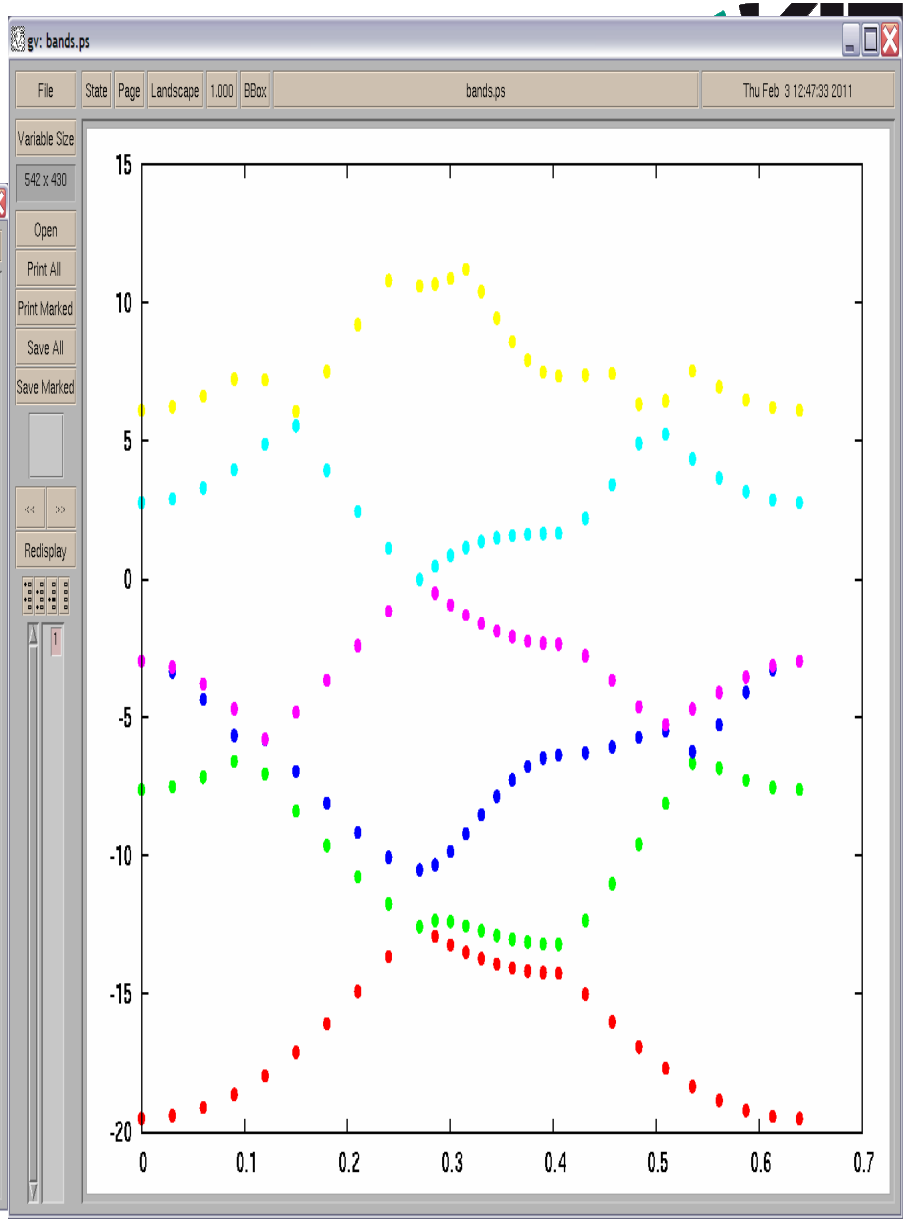
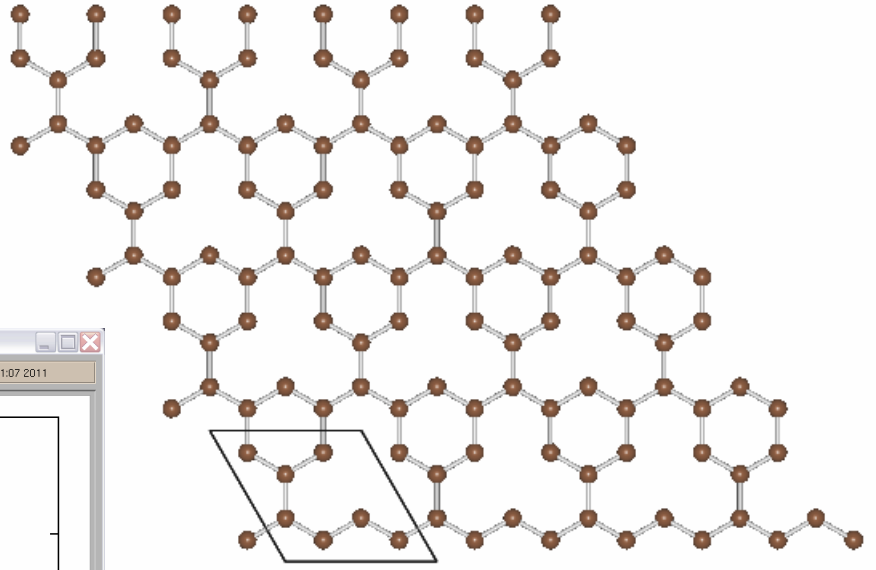
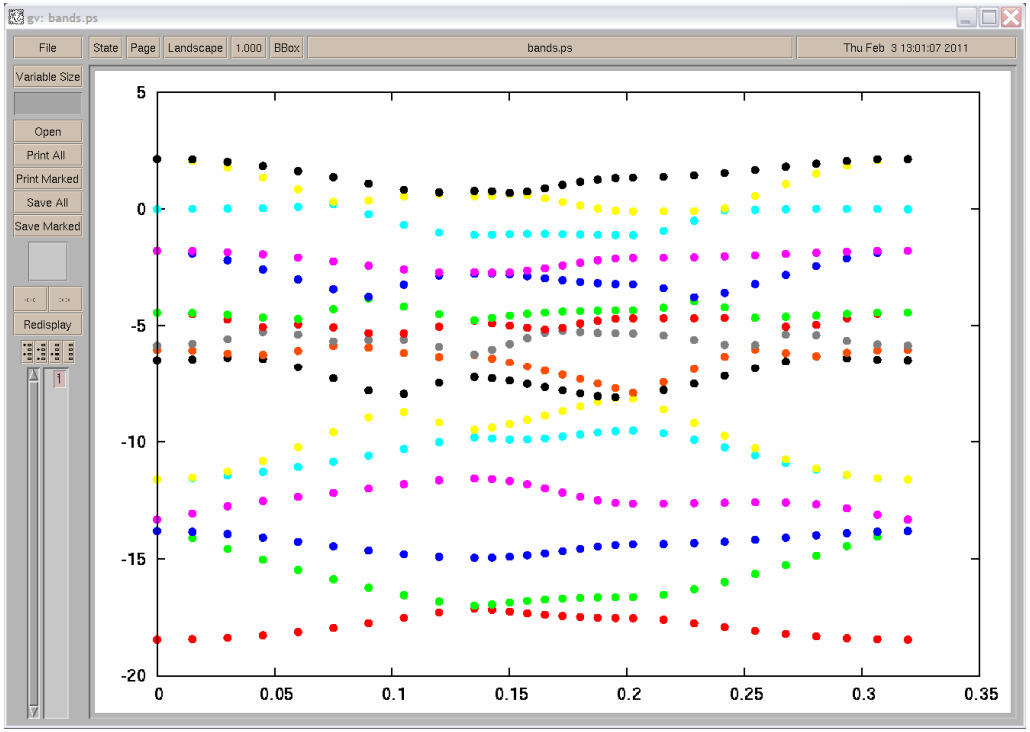




02 C vacancy




gv: bands.ps
File
State
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1.000
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bands.ps
Thu Feb 3 13:01:07 2011
Variable Size
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Print All
Print Marked
Save All
Save Marked
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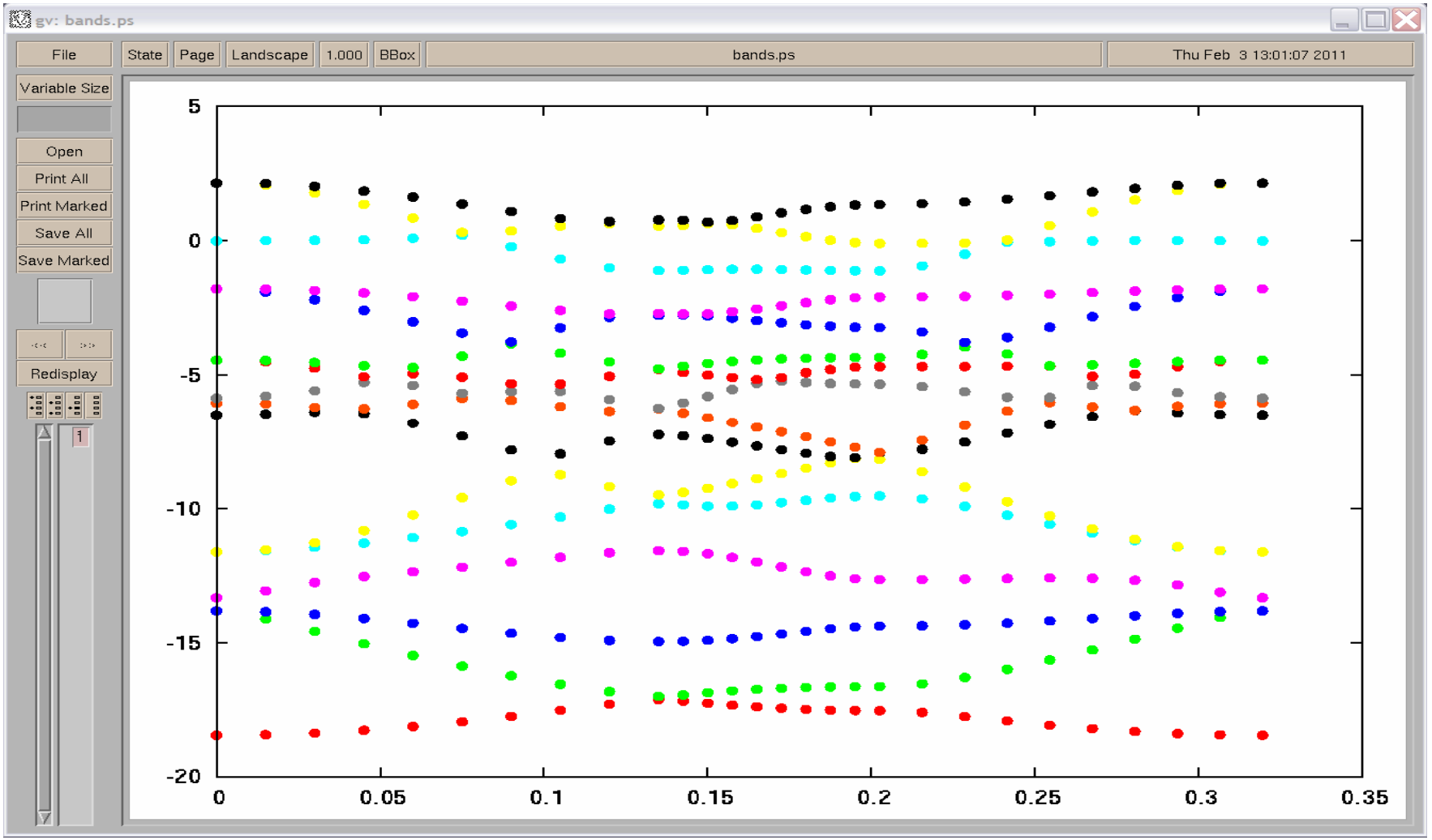
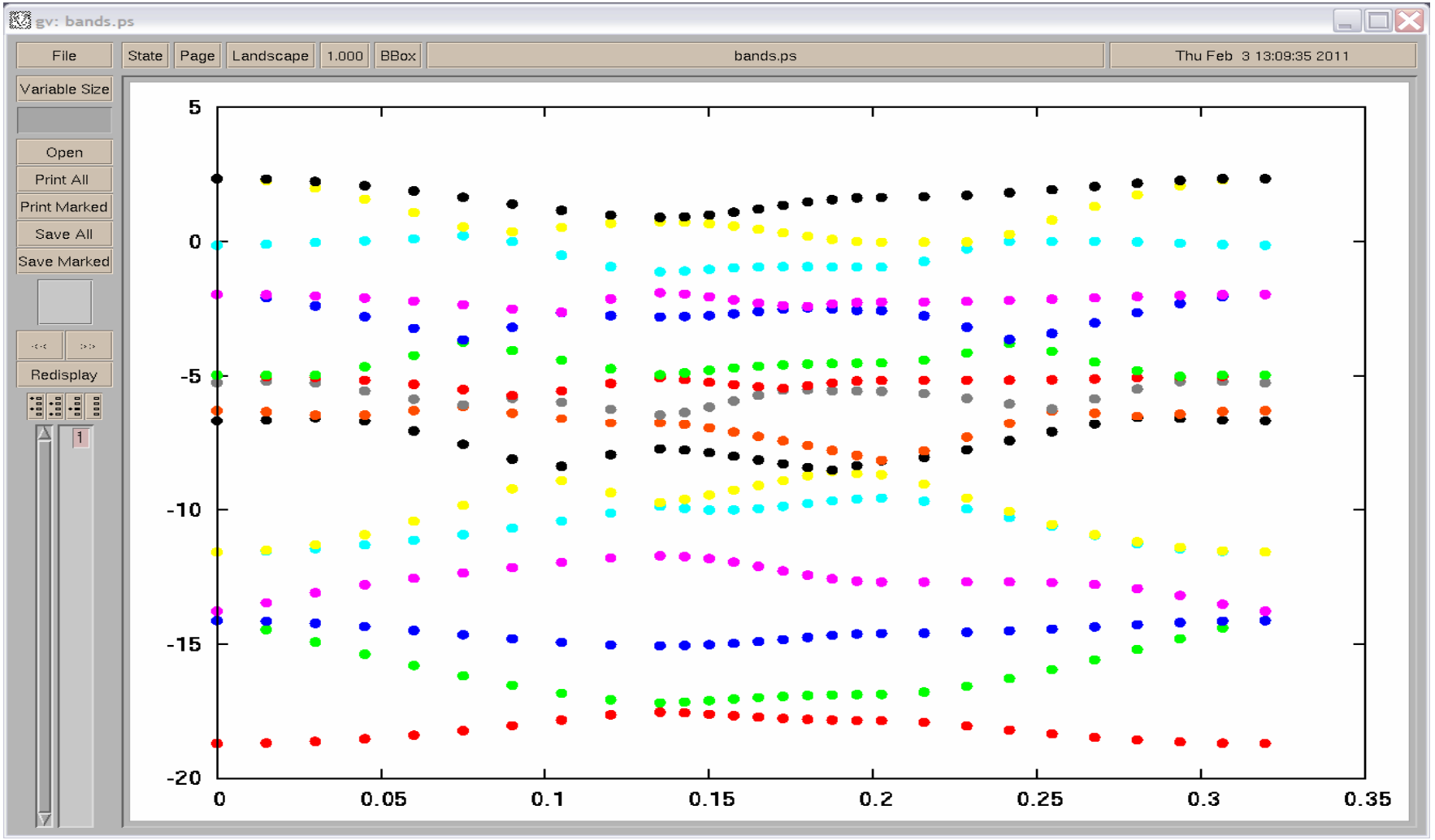
-5
-10
-15
-20
0
0.05
0.1
0.15
0.2
0.25
0.3
0.35

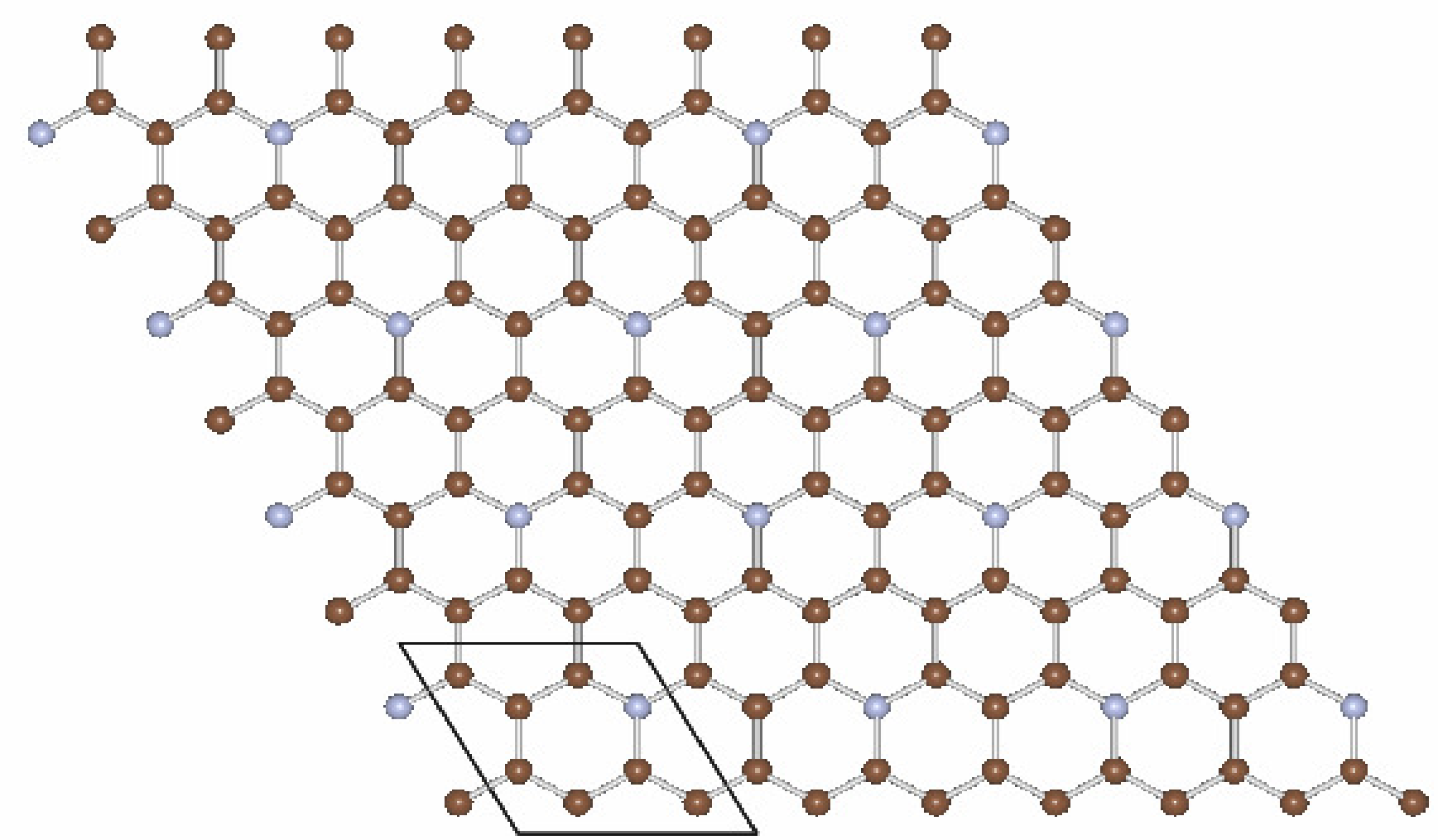
02 C vacancy: Unrelaxed



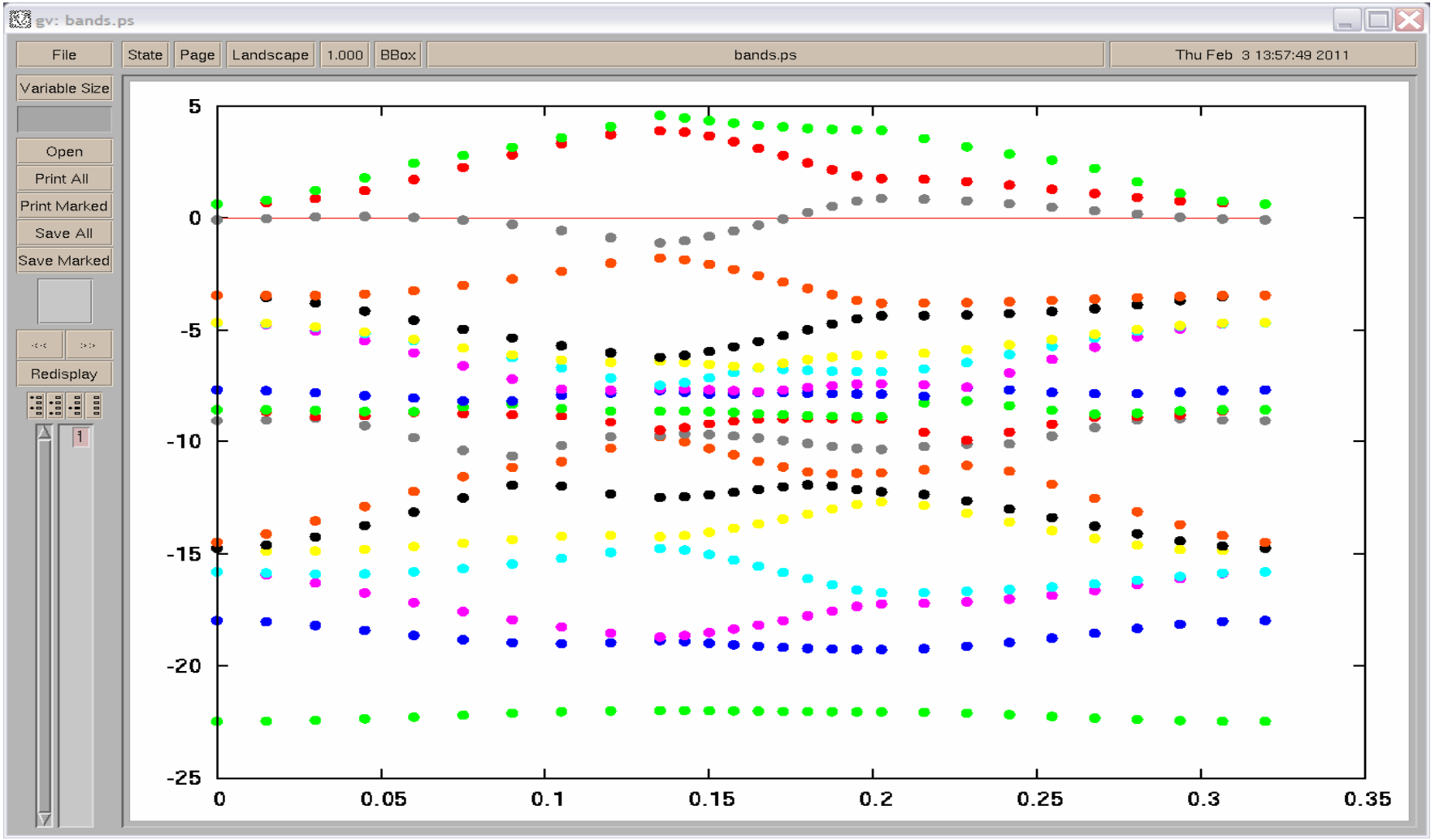
02 C vacancy: Relaxed



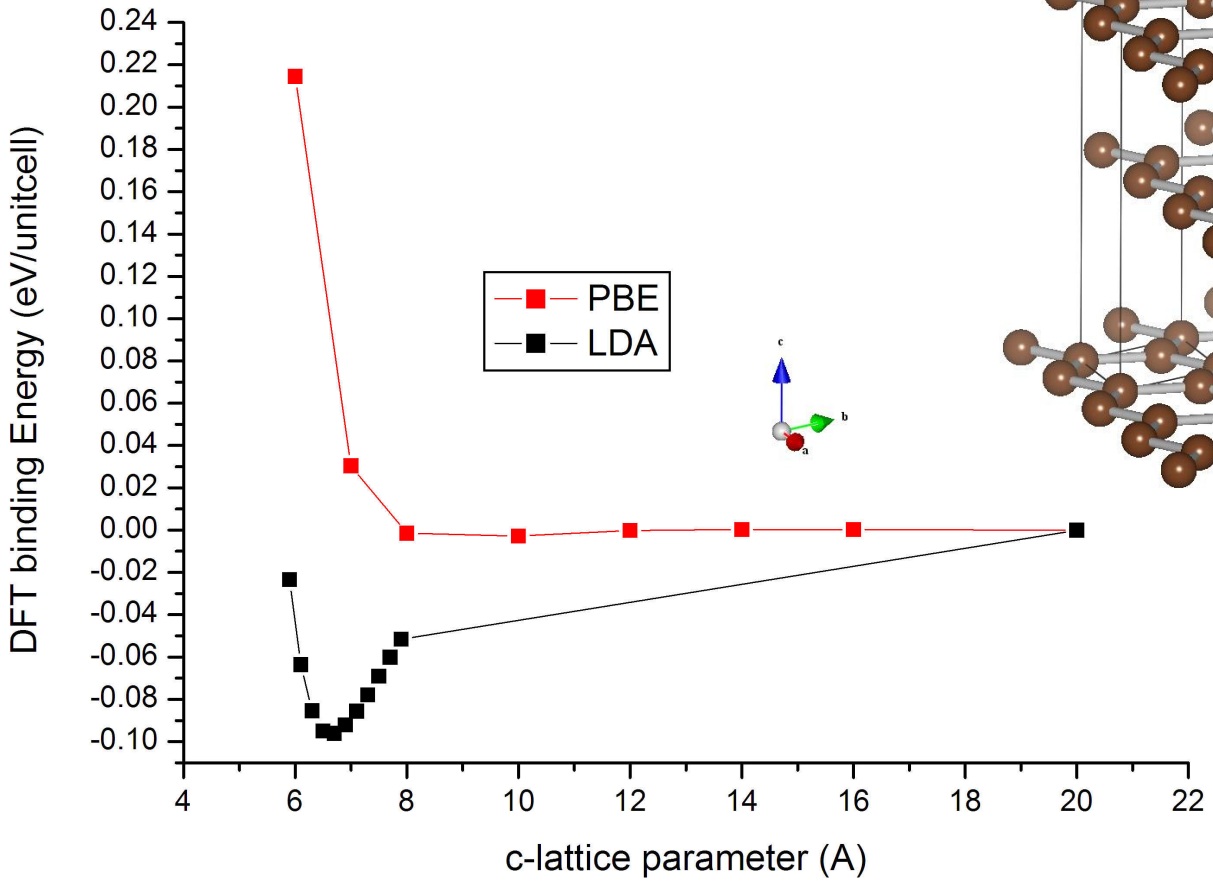
02 N-defect

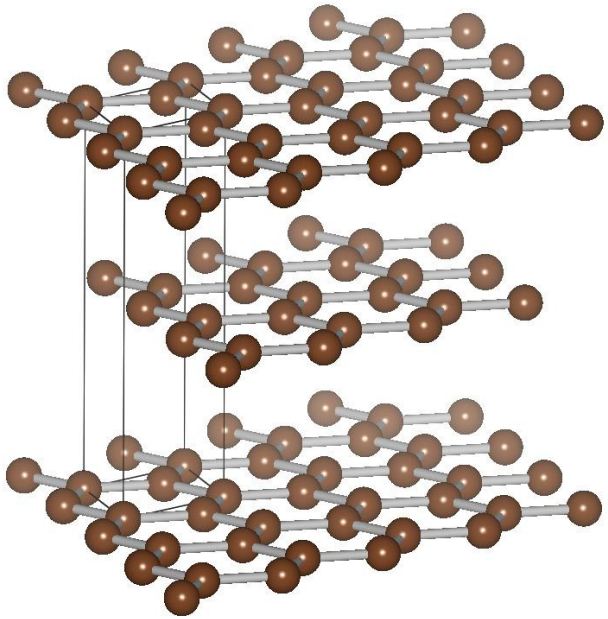


02 N defect: Unrelaxed



Graphite c-lattice parameter





Layered structures: Mg(AlH4)2 example

- What goes wrong in optimizing the structure

	exp	2005 paper	normal	Mg_pv	H_h
		PW91	PBE		
			gamma 10 10 10		
			accurate, aspherical correction, ltb		
encut			250	400	700
volume	137.2837	143.0774	145.6802	145.8290	144.5964
		4.22	6.12	6.22	5.33
a	5.2100	5.2300	5.2584	5.2567	5.2512
		0.38	0.93	0.90	0.79
c	5.8400	6.0400	6.0835	6.0938	6.0549
		3.42	4.17	4.35	3.68
Al_z	0.6990	0.7060	0.7070	0.7079	0.7072
		1.00	1.15	1.28	1.18
H1_z	0.4240	0.4420	0.4428	0.4447	0.4423
		4.25	4.43	4.89	4.32
H2_x	0.1670	0.1680	0.1681	0.1683	0.1682
		0.60	0.68	0.80	0.70
H2_z	0.8110	0.8120	0.8120	0.8127	0.8123
		0.12	0.12	0.22	0.16

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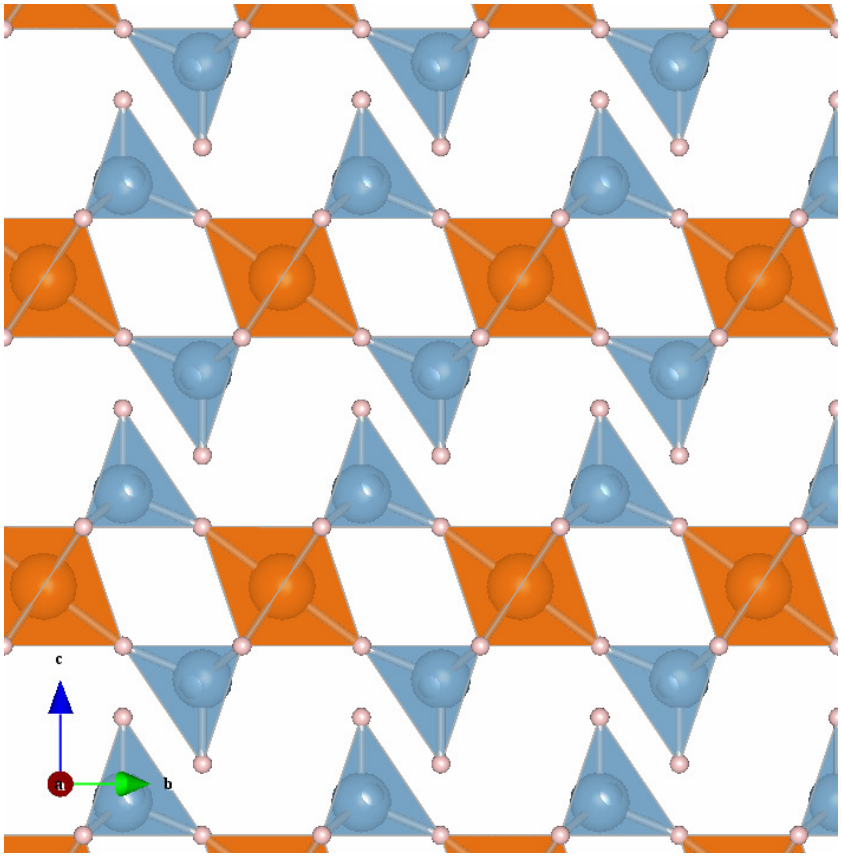
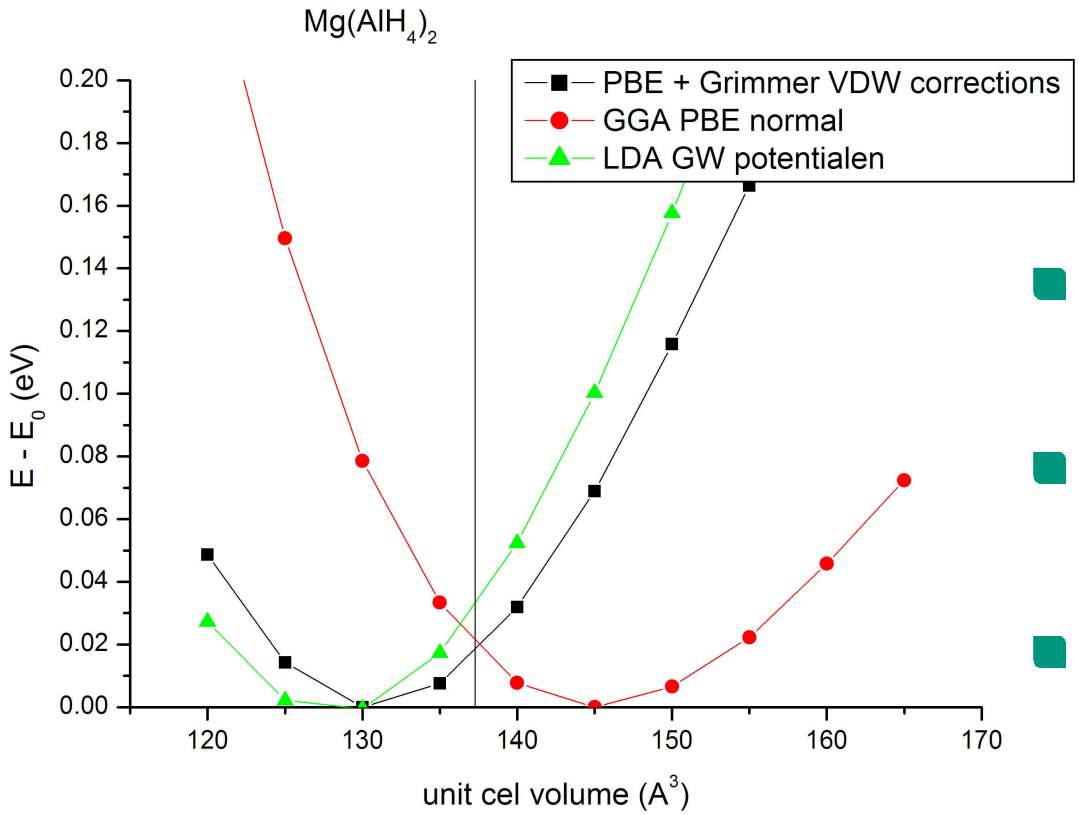


- Layered structure….

$Mg(AlH_4)_2$ different XC potentials



- GGA underbinds
- LDA overbinds
- Simple VdW correction is not much better…