KATILARIN ELEKTRONİK YAPISININ BENZETİŞİMİ

Yoğun Madde Fiziğinde Kullanılan Yazılımlardan ab-initio Tekniği-2

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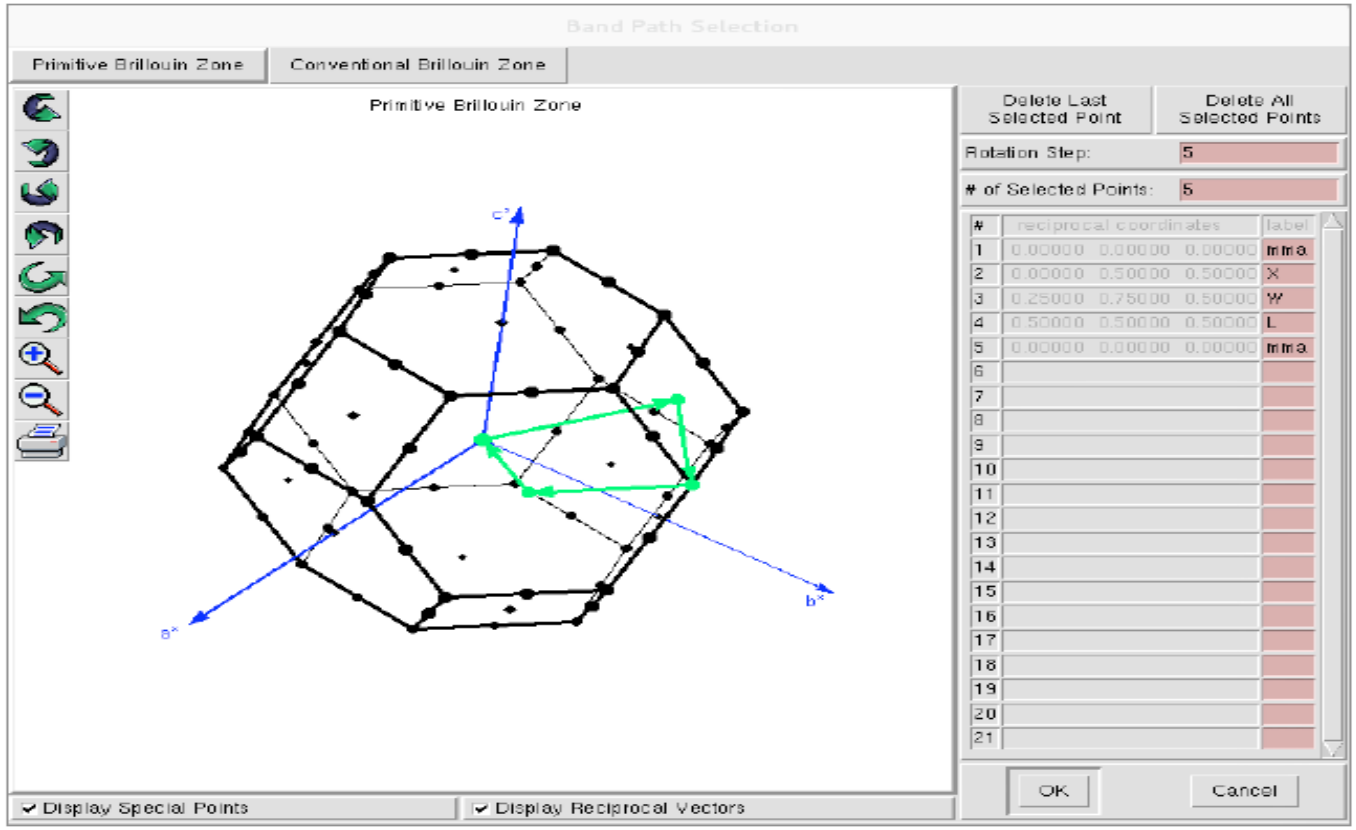
Hafta	DERS İÇERİĞİ
1.	Malzeme Bilimi: Temel Kavramlar
2.	**Yoğun Madde Fiziğinde Kullanılan Yazılımlardan ab-initio Tekniği**
3.	Kristal Fiziği: Temel Kavramlar-1
4.	Kristal Fiziği: Temel Kavramlar-2
5.	Katıların Bant Teorisi
6.	Elektronik Bant Yapıları: İletkenlik durumları
7.	VİZE SINAVI

Hafta	DERS İÇERİĞİ
8.	Durum Yoğunlukları ve Fermi Yüzeyleri
9.	Katıların Elastik Özellikleri: Elastik sabitleri, Young, Shear Modülleri..
10.	Katıların Optik Özellikleri: Dielektrik sabitleri, Yansıma, soğurma, sönüm katsayıları, kırılma indisi
11.	Katıların Titreşimsel Özellikleri: Fononlar
12.	Kristal yapının programlama yardımıyla kurulması
13.	Katının elektronik bant yapısının programlama yardımıyla çizdirilmesi
14.	FİNAL SINAVI

KPOINTS



K-Points mesh generation
Using X-CrysDen

KPOINTS

KPOINTS (1)

There are 3 ways to prepare a KPOINTS file:

- Entering all k-points explicitly
- Strings of k-points for band structure calculations ← For band structure calculation.
- Automatic k-mesh generation

In most cases, doing optimization, prepare a CHGCAR ...

- Automatic k-mesh generation

```
Automatic Generation
 0                    number of k-points = 0 ->automatic generation scheme
Gamma                 Gamma ! generate a Gamma centered grid
  9   9   1           subdivisions N_1, N_2 and N_3 along reciprocal vectors
0.0 0.0 0.0           optional shift of the mesh (s_1, s_2, s_3)
```

KPOINTS

KPOINTS (2)

- Automatic k-mesh generation

  The Gamma can be replaced by Monkhorst. The difference is

In Gamma case,

$$\vec{k} = \vec{b}_1 \frac{n_1 + s_1}{N_1} + \vec{b}_2 \frac{n_2 + s_2}{N_2} + \vec{b}_3 \frac{n_3 + s_3}{N_3}.$$

In Monkhorst case,

$$\vec{k} = \vec{b}_1 \frac{n_1 + s_1 + 1/2}{N_1} + \vec{b}_2 \frac{n_2 + s_2 + 1/2}{N_2} + \vec{b}_3 \frac{n_3 + s_3 + 1/2}{N_3}.$$

POTCAR

POTCAR (1)

The pseudopotential for each atomic species are in data base at some where in c238. Basically, If your system has many type of atom species, you need to concat them in one file with name of POTCAR. The sequence is important and needs to be the same as in POSCAR.

There are two type of POTCAR flavors: (i) Ultra-soft (ii) PAW (projected augmented wave). The 2nd one is more popular now.

In POTCAR, the information of ENMAX is written in, which can be used for ENCUT.

POTCAR

POTCAR (2)

```
PAW C 31May2000
4.00000000000000000
parameters from PSCTR are:
  VRHFIN =C: s2p2
  LEXCH  = CA
  EATOM  =   146.6877 eV,   10.7812 Ry

  TITEL  = PAW C 31May2000
  LULTRA =       F    use ultrasoft PP ?
  IUNSCR =       0    unscreen: 0-lin 1-nonlin 2-no
  RPACOR =    .000    partial core radius
  POMASS =  12.011; ZVAL   =    4.000    mass and valenz
  RCORE  =   1.500    outmost cutoff radius
  RWIGS  =   1.630; RWIGS  =    .863    wigner-seitz radius (au A)
  ENMAX  = 400.000; ENMIN  =  300.000 eV
  ICORE  =       2    local potential
  LCOR   =       T    correct aug charges
  LPAW   =       T    paw PP
  EAUG   =  644.873
  DEXC   =    .000
  RMAX   =   2.266    core radius for proj-oper
  RAUG   =   1.300    factor for augmentation sphere
  RDEP   =   1.501    radius for radial grids
  RDEPT  =   1.300    core radius for aug-charge
  QCUT   =  -5.516; QGAM   =   11.032    optimization parameters
```

SOME CALCULATIONS

What is the primitive lattice constant after relaxation? (Check POSCAR after complete relaxation).
When you change kpoints and encut, how does it change?
How does E0 at the end of relaxation (in file OSZICAR after relaxation is complete) change with kpoints and encut?

Graphene

Change of lattice constant after relaxation w.r.t. kpoints and encut

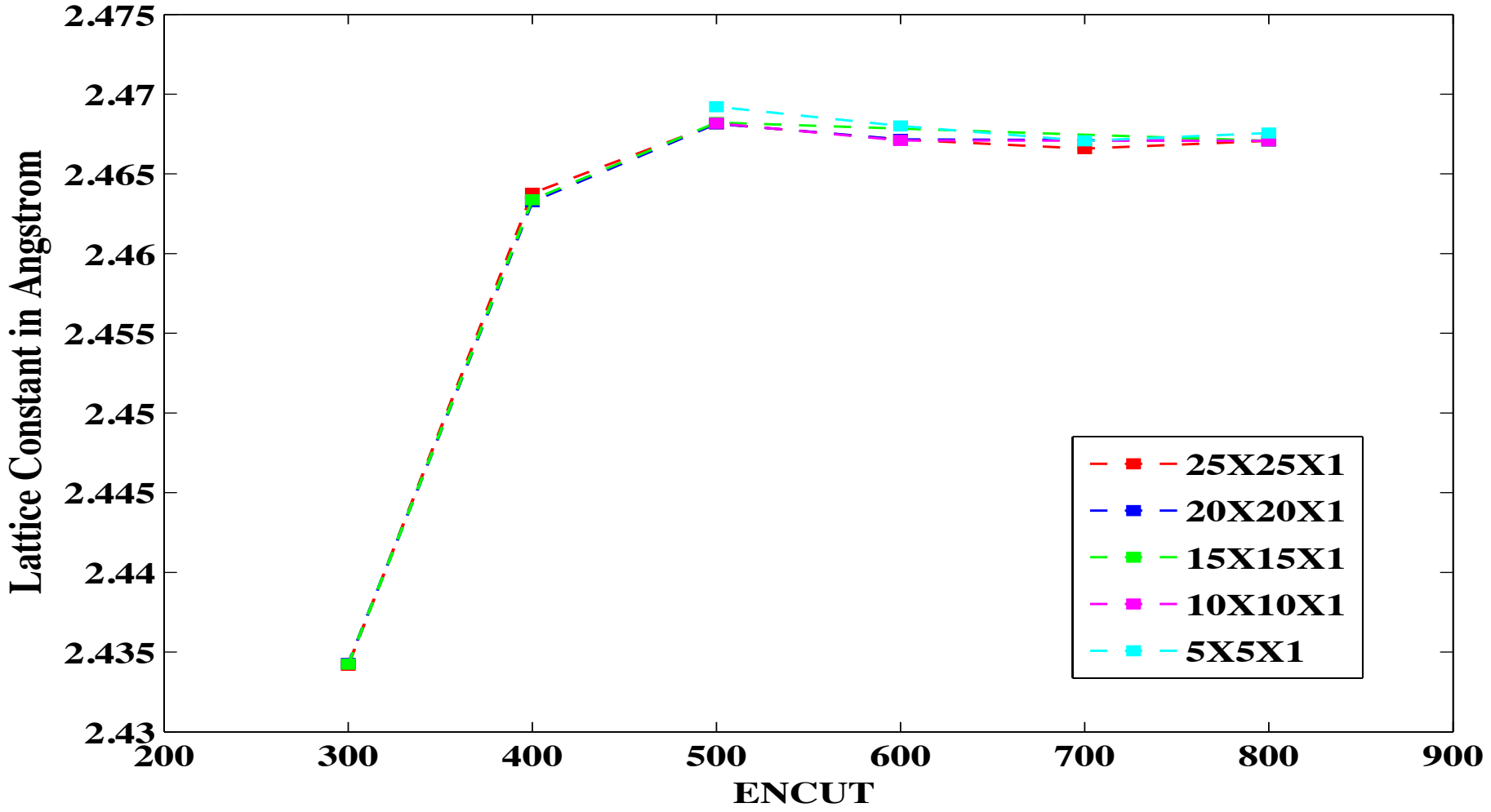
Lattice constant after relaxation (for kpoints : 25 X 25 X 1 and encut : 800) :: 2.4670806653457333

kpoints	encut					
	800	700	600	500	400	300
25X25X1	2.4670806653457333	2.4665871522083092	2.4671571110173507	2.4681418256445364	2.4637852449228284	2.4341658373949655
20X20X1	2.4670806653457333	-	2.4671622581862587	2.4681466378326493	2.4632578609573628	2.4342858693118195
15X15X1	2.4670806653457333	-	-	2.4682248606386414	2.4633795149699513	2.4342381704326046
10X10X1	2.4670806653457333	-	2.4670927951197861	2.4681737723293224	-	2.4343573743232945
5X5X1	2.4675658851610760	2.4670806653457333	2.4680056983693262	2.4692106733146226	-	2.4340396306444076

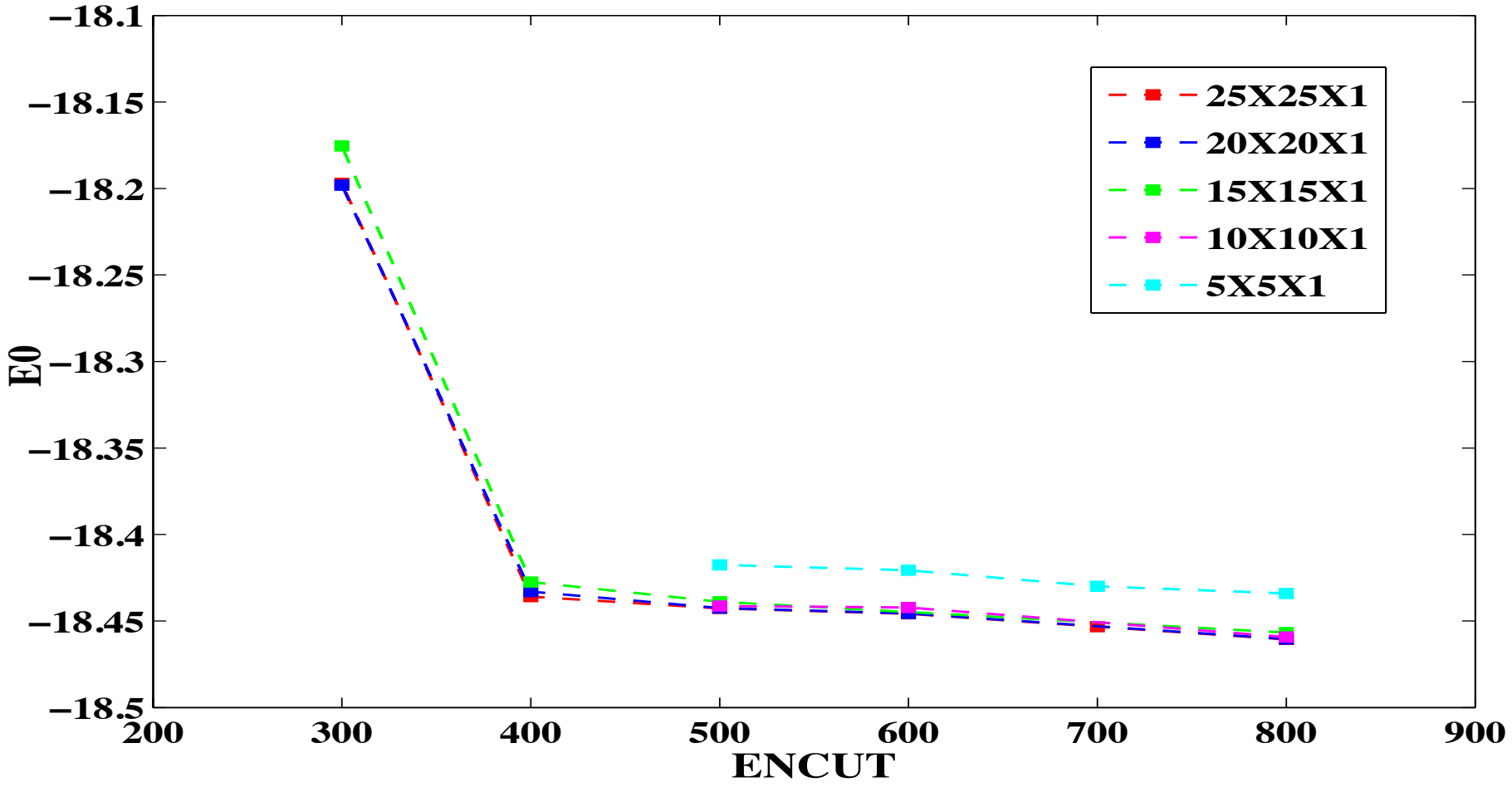
Change of E0 after relaxation w.r.t. kpoints and encut

kpoints	encut					
	800	700	600	500	400	300
25X25X1	-.18460600E+02	-.18453275E+02	-.18445805E+02	-.18442708E+02	-.18435830E+02	-.18197038E+02
20X20X1	-.18460371E+02	-	-.18445552E+02	-.18442482E+02	-.18432960E+02	-.18198179E+02
15X15X1	-.18456681E+02	-	-	-.18438870E+02	-.18427417E+02	-.18175421E+02
10X10X1	-.18459185E+02	-	-.18442154E+02	-.18441298E+02	-	-.18193576E+02
5X5X1	-.18434049E+02	-.18429871E+02	-.18420666E+02	-.18417521E+02	-	-.18074892E+02

Variation of lattice constant w.r.t. kpoints & encut



Variation of E0 w.r.t. kpoints & encut



THANK YOU.