KATILARIN ELEKTRONİK YAPISININ BENZETİŞİMİ

Yoğun Madde Fiziğinde Kullanılan Yazılımlardan ab-initio Tekniği-3

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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

Convergence Test

Once the relaxation is complete with high kpoints and high cutoff, then do only single point calculations as follows:

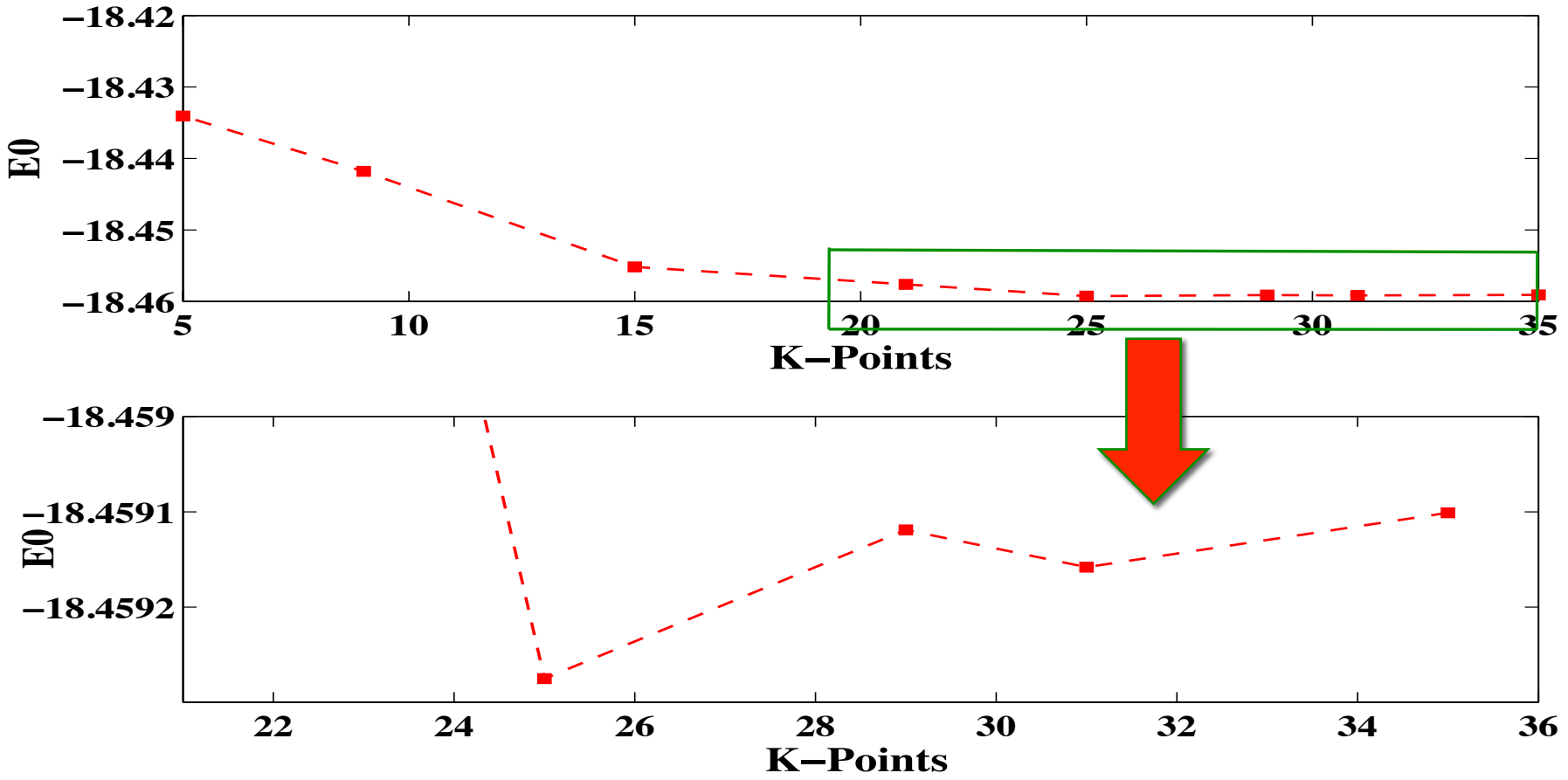
a) Fix encut to 800 eV (in incar). Gradually vary kpoints (in kpoints) from 25x25x1 to 5x5x1. Plot E0 (in OSZICAR) vs kpoints.

b) Fix kpoints to 25x25x1. Vary encut from 300 eV to 800 eV in steps of 50. Plot E0 vs encut.

Identify optimum kpoints and encut for this material.

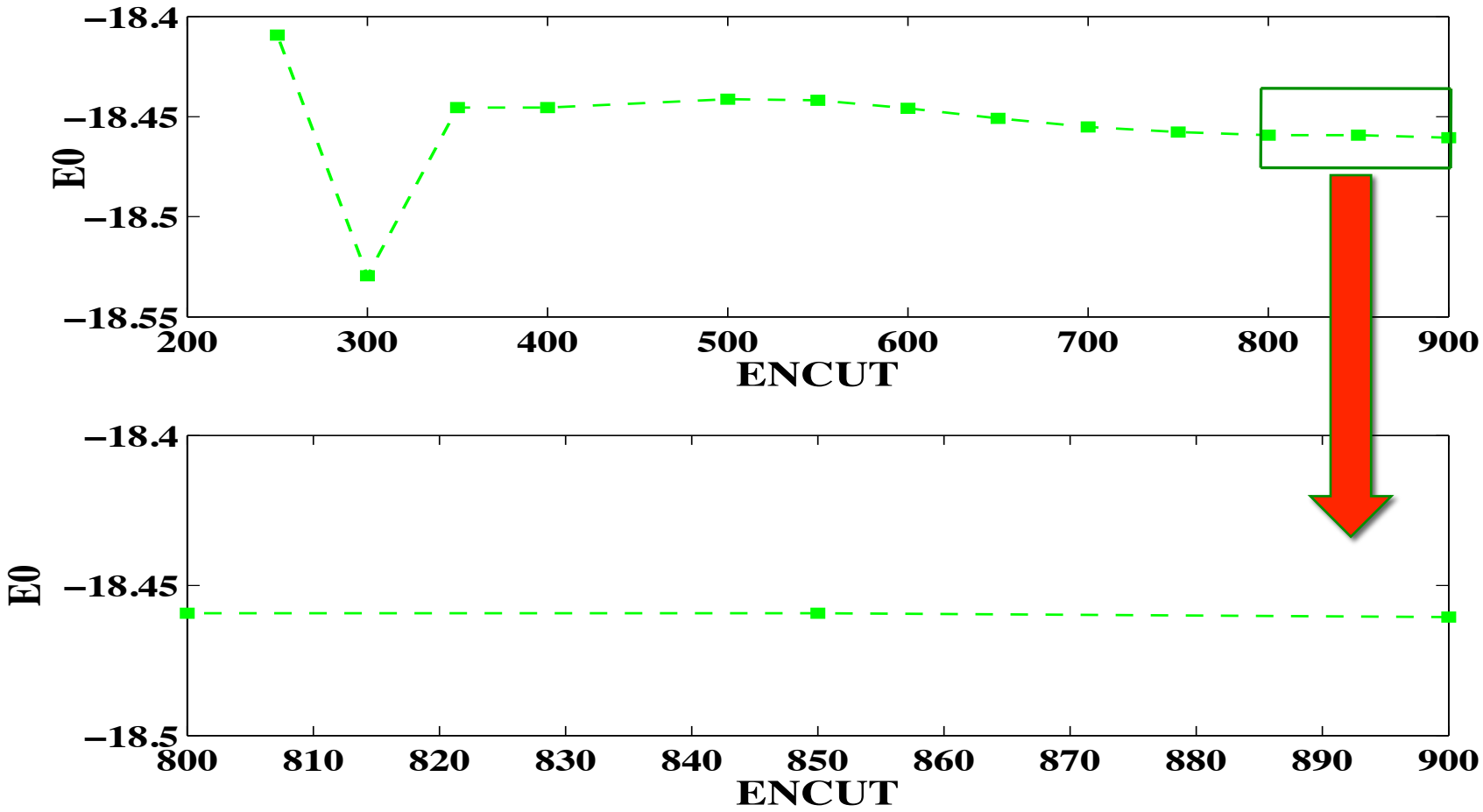
Graphene

	K-points							
	5X5	11X11	15X15	21X21	25X25	29X29	31X31	35X35
E0	-.18434067E+02	-.18441804E+02	-.18455182E+02	-.18457623E+02	-.18459275E+02	-.18459119E+02	-.18459158E+02	-.18459101E+02



Graphene

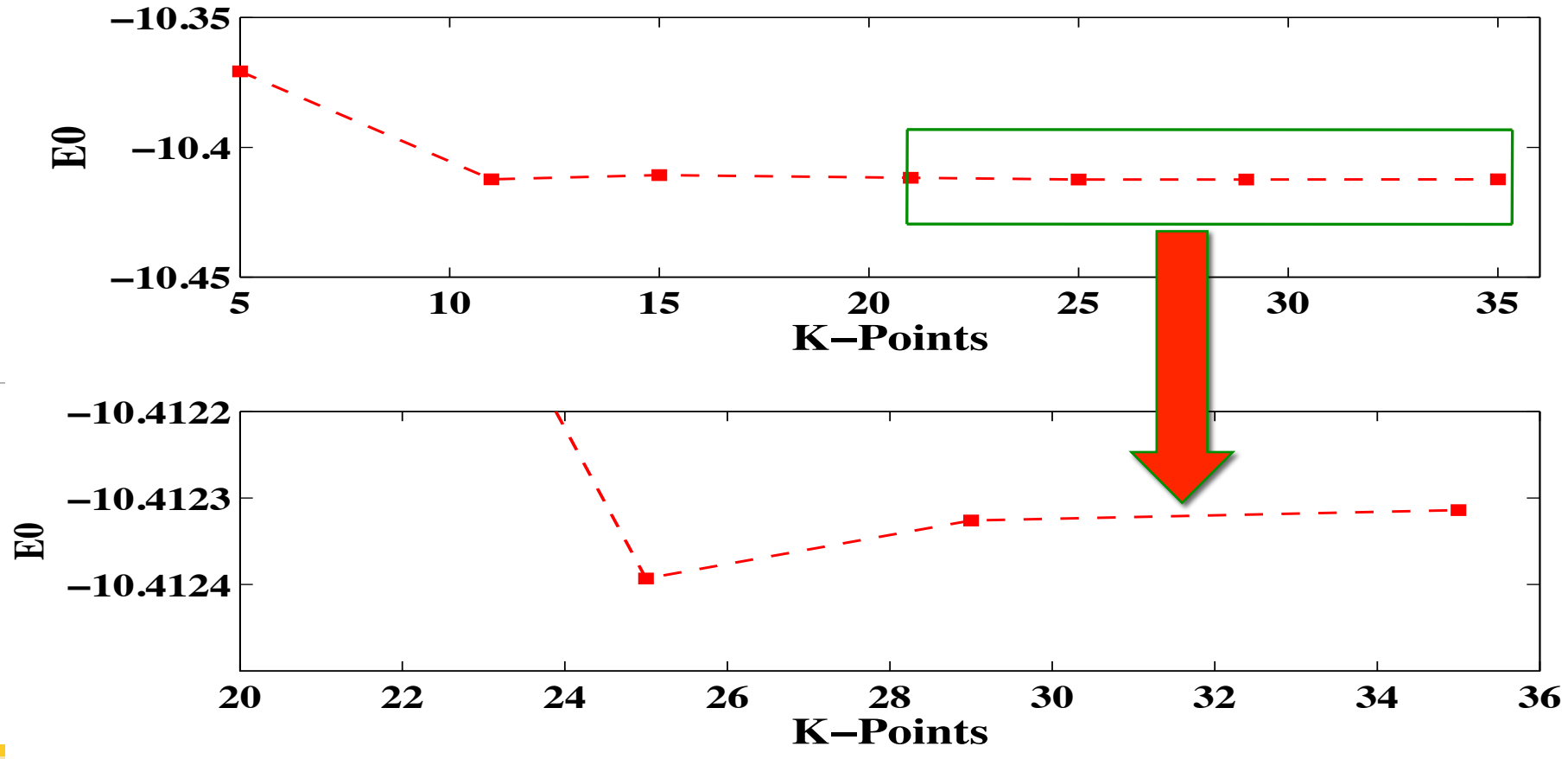
Encut	E0
900	-.18460503E+02
850	-.18459275E+02
800	-.18459275E+02
750	-.18457712E+02
700	-.18455141E+02
650	-.18450863E+02
600	-.18445870E+02
550	-.18441799E+02
500	-.18441325E+02
450	-.18445504E+02
400	-.18445504E+02
350	-.18484323E+02
300	-.18529555E+02
250	-.18409306E+02



Optimum K-Points : 25X25X1 ; Optimum ENCUT : 800

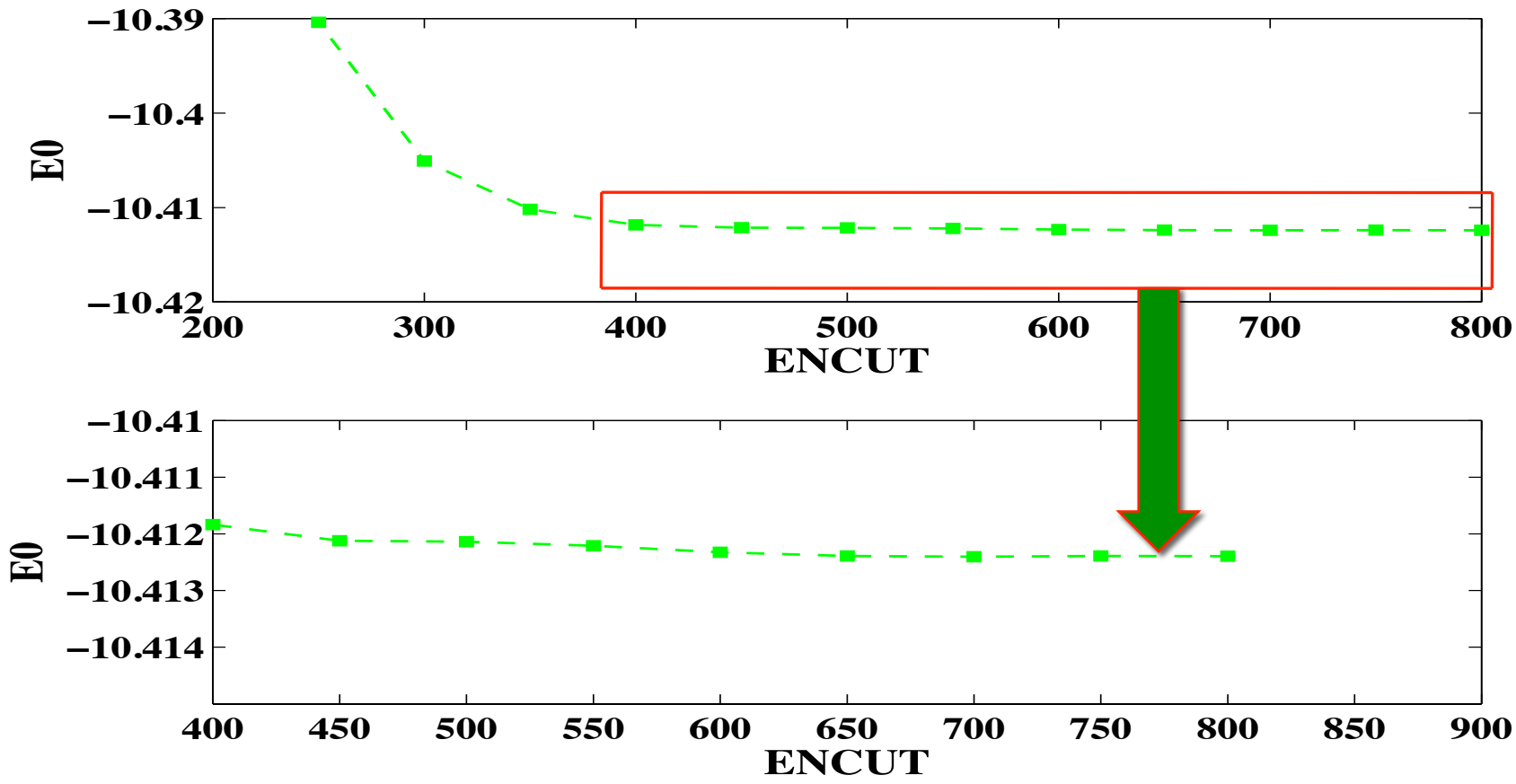
Silicene

	K-points						
	5X5	11X11	15X15	21X21	25X25	29X29	35X35
E0	-.10370682E+02	-.10412261E+02	-.10410677E+02	-.10411698E+02	-.10412393E+02	-.10412326E+02	-.10412314E+02



Silicene

encut	E0
800	-.10412393E+02
750	-.10412391E+02
700	-.10412404E+02
650	-.10412390E+02
600	-.10412324E+02
550	-.10412211E+02
500	-.10412138E+02
450	-.10412120E+02
400	-.10411837E+02
350	-.10410181E+02
300	-.10405066E+02
250	-.10390390E+02



Optimum K-Points : 25X25X1 ; Optimum ENCUT : 500 eV

Charge Density

For the relaxed structure and with optimum kpoints and encut, do a single point calculation.

Plot charge density using VESTA (charge density is written in CHGCAR.2, use this file along with OUTCAR.2 in VESTA). Plot the charge density such that I can clearly see sigma (inplane C-C) orbitals and pi orbitals (out-of-plane). Increase the density of kpoints mesh and replot charge density.

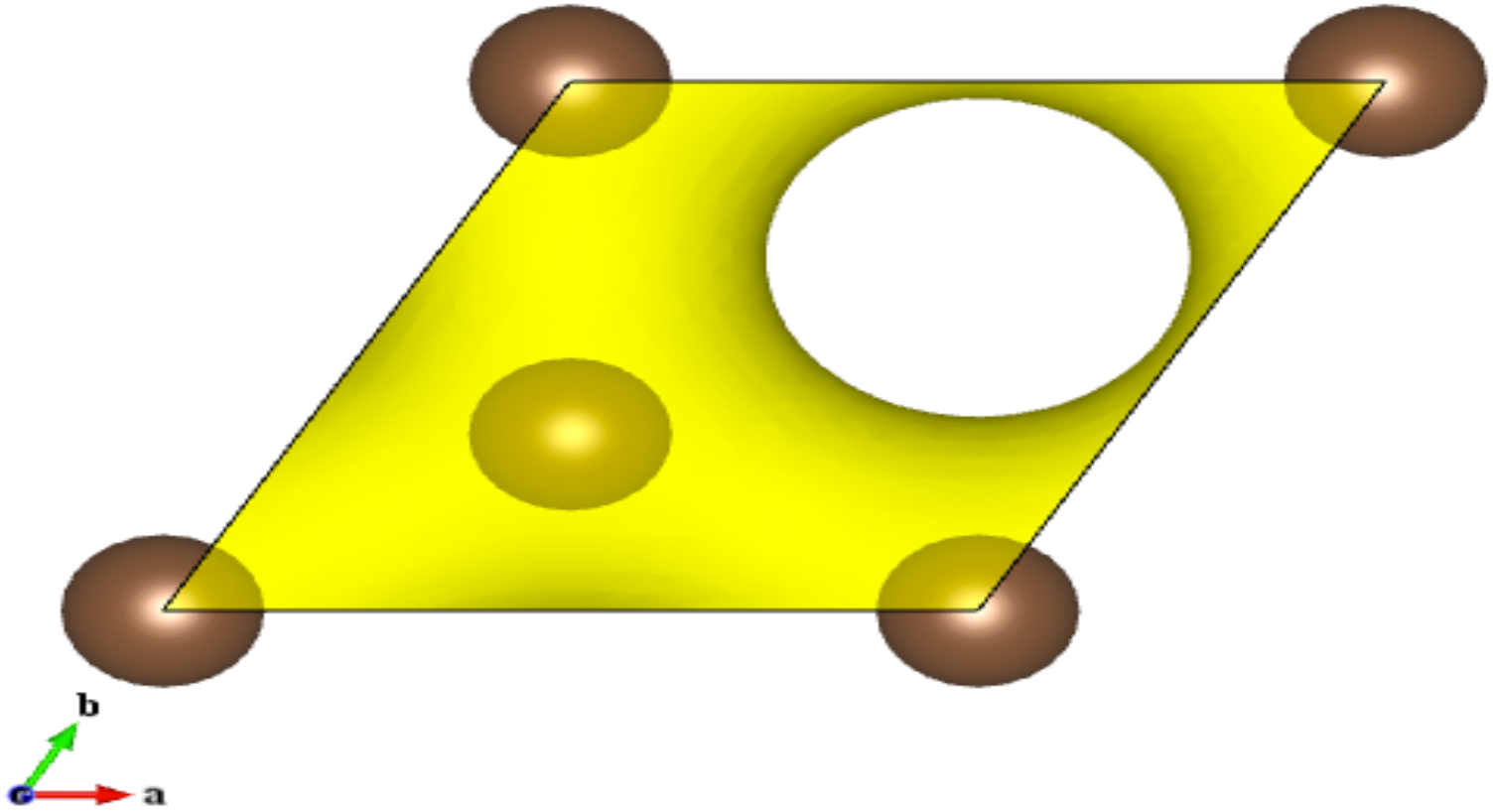
Integrate charge density on each atom using bader analysis.

How many electrons does each atom have?

Graphene

Charge Density with optimum kpoints and encut

K-Points : 25X25X1



Graphene

Bader Analysis

#	X	Y	Z	CHARGE	MIN DIST	ATOMIC VOL
1	1.2335	0.7122	7.0000	3.8211	0.5087	37.0103
2	0.0000	0.0000	7.0000	4.1789	0.6168	36.7844

VACUUM CHARGE: 0.0000
VACUUM VOLUME: 0.0000
NUMBER OF ELECTRONS: 8.0000

Density of States

Where is the Fermi level? Plot density of states from DOSCAR.2.
Split DOSCAR.2 for density of states integrated on each atom.

Plot total DOS for spin up and spin down channels.

Plot integrated DOS for two channel.

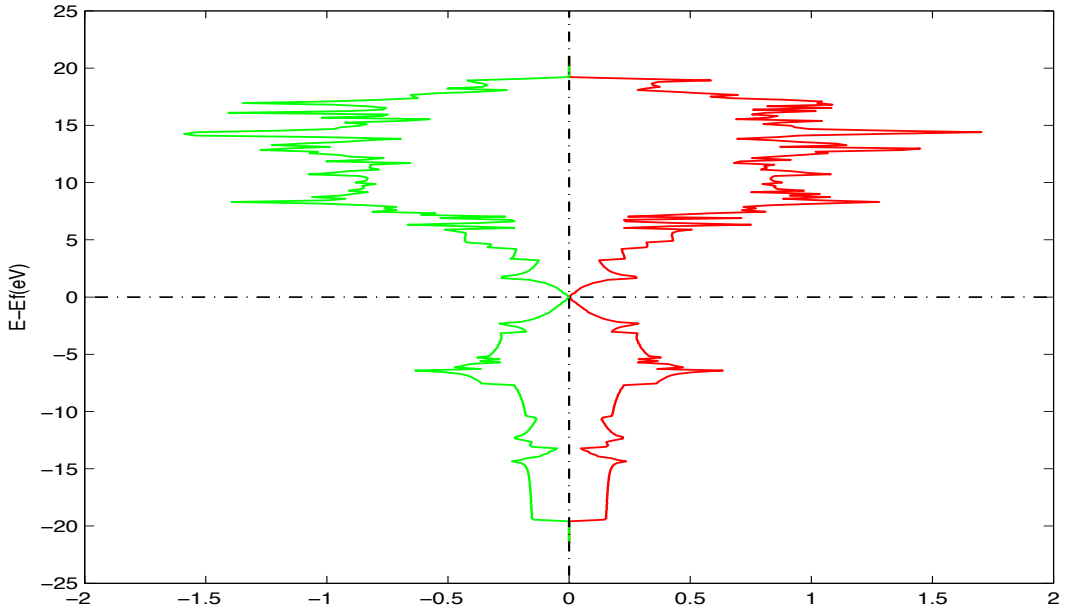
Plot partial density of states for s, p, d, f orbitals, for both spin-up and spin-down.

Graphene

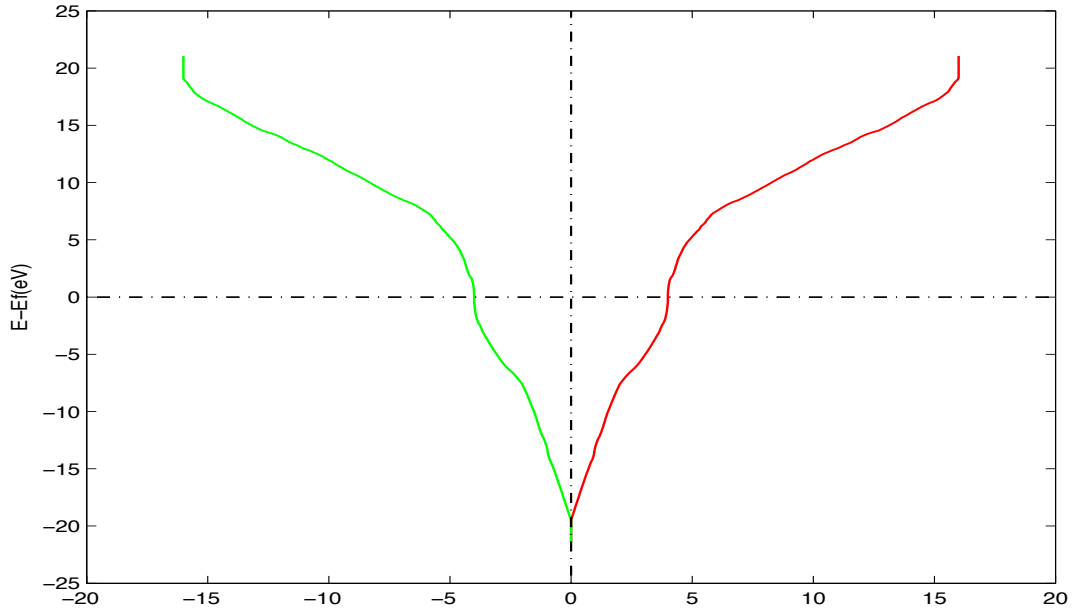
Total DOS

Blochl-tetrahedron smearing

DOS for Spin Up & Down



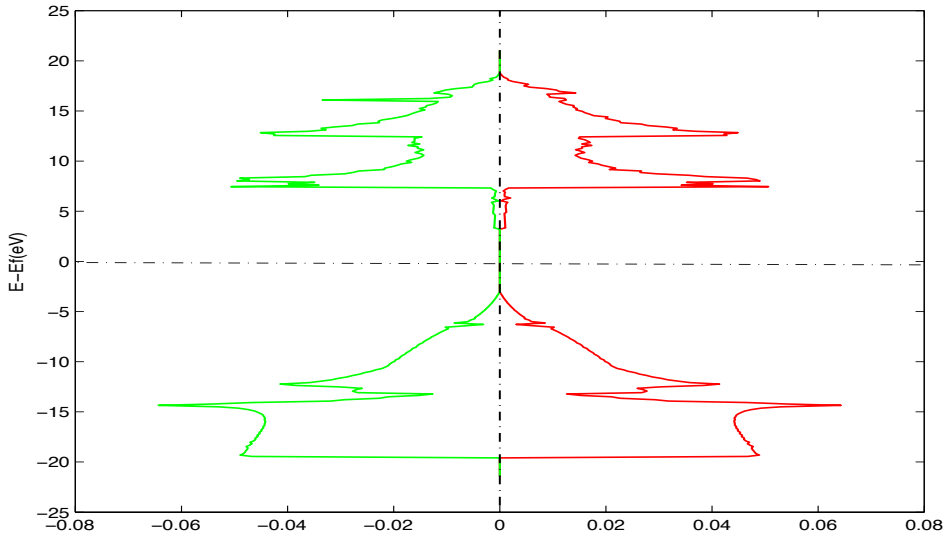
Integrated DOS for Spin Up & Down



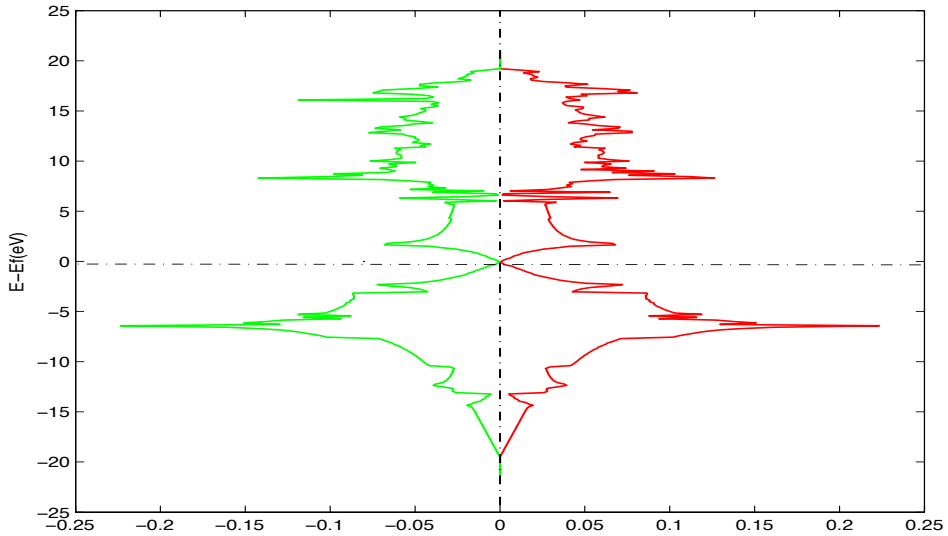
K Points : 45X45X1 , ENCUT : 600 eV

Total DOS

S- orbital



P - orbital

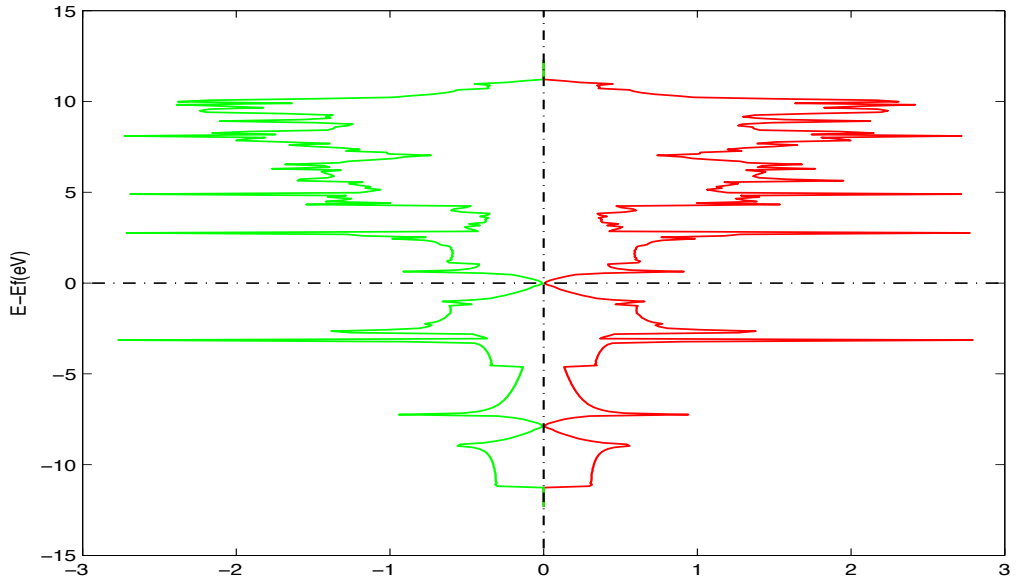


K Points : 45X45X1 ; ENCUT : 600 eV

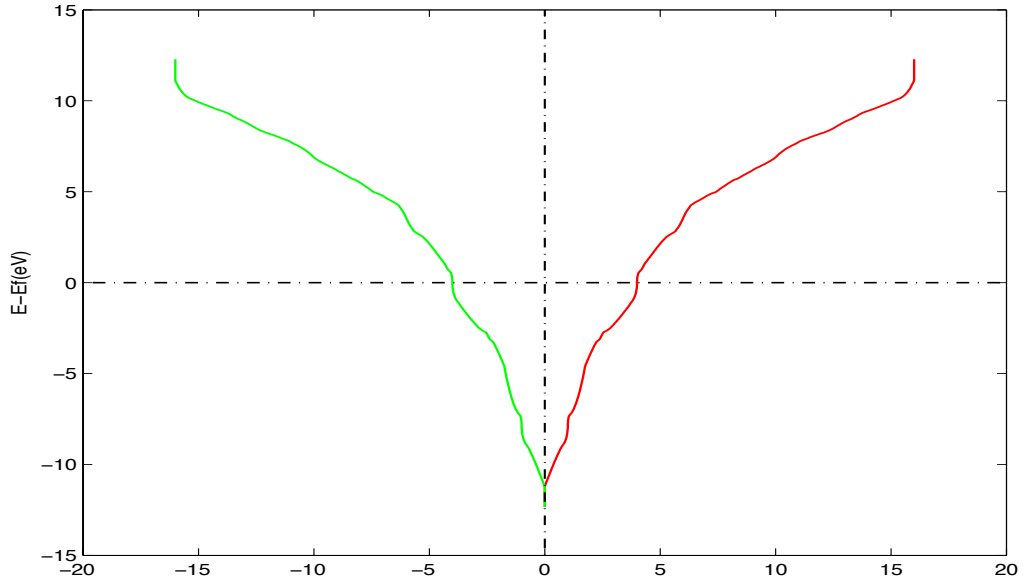
Silicene

Total DOS

DOS for Spin Up & Down



Integrated DOS for Spin Up & Down

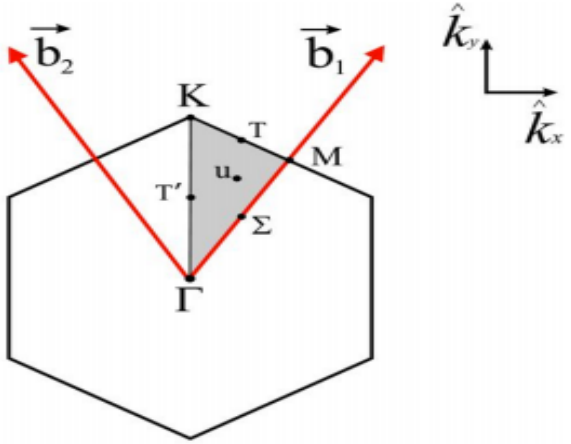


K Points : 45X45X1 , ENCUT : 600 eV

Graphene

First Brillouin Zone

First Brillouin zone (BZ)



$$\vec{b}_1 = \frac{2\pi}{a}\left(\frac{\sqrt{3}}{3}\hat{k}_x + \hat{k}_y\right)$$

$$\vec{b}_2 = \frac{2\pi}{a}\left(-\frac{\sqrt{3}}{3}\hat{k}_x + \hat{k}_y\right)$$

#kpoints for bandstructure of graphene
10
Line-modereciprocal
0.0 0.0 0.0 ! \Gamma
0.6667 0.3333 0.0 ! K

0.6667 0.3333 0.0 ! K
0.50 0.0 0.0 ! M

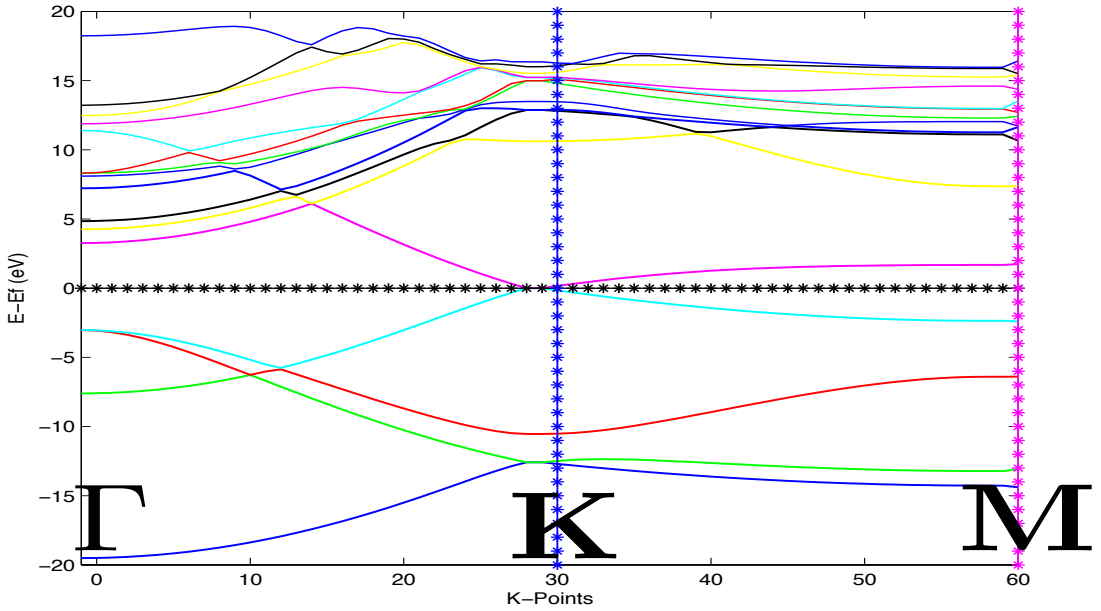
0.50 0.0 0.0 ! M
0.0 0.0 0.0 ! \Gamma

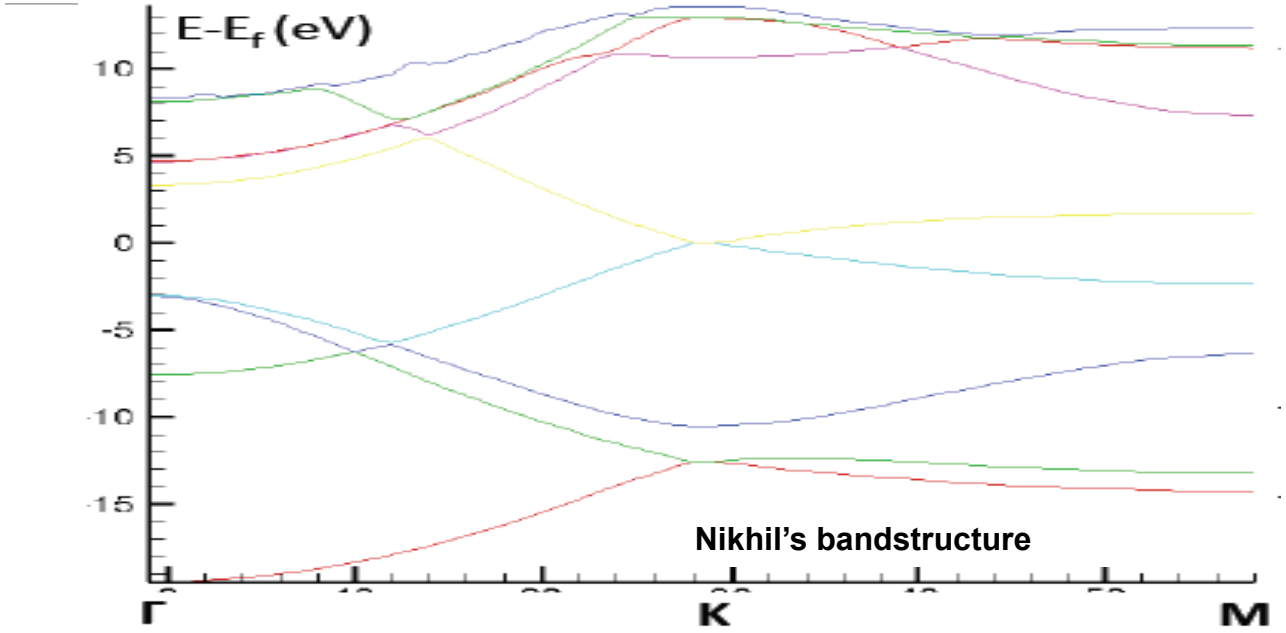
Graphene

Band Structure Plot

Blochl-tetrahedron smearing

Spin Up



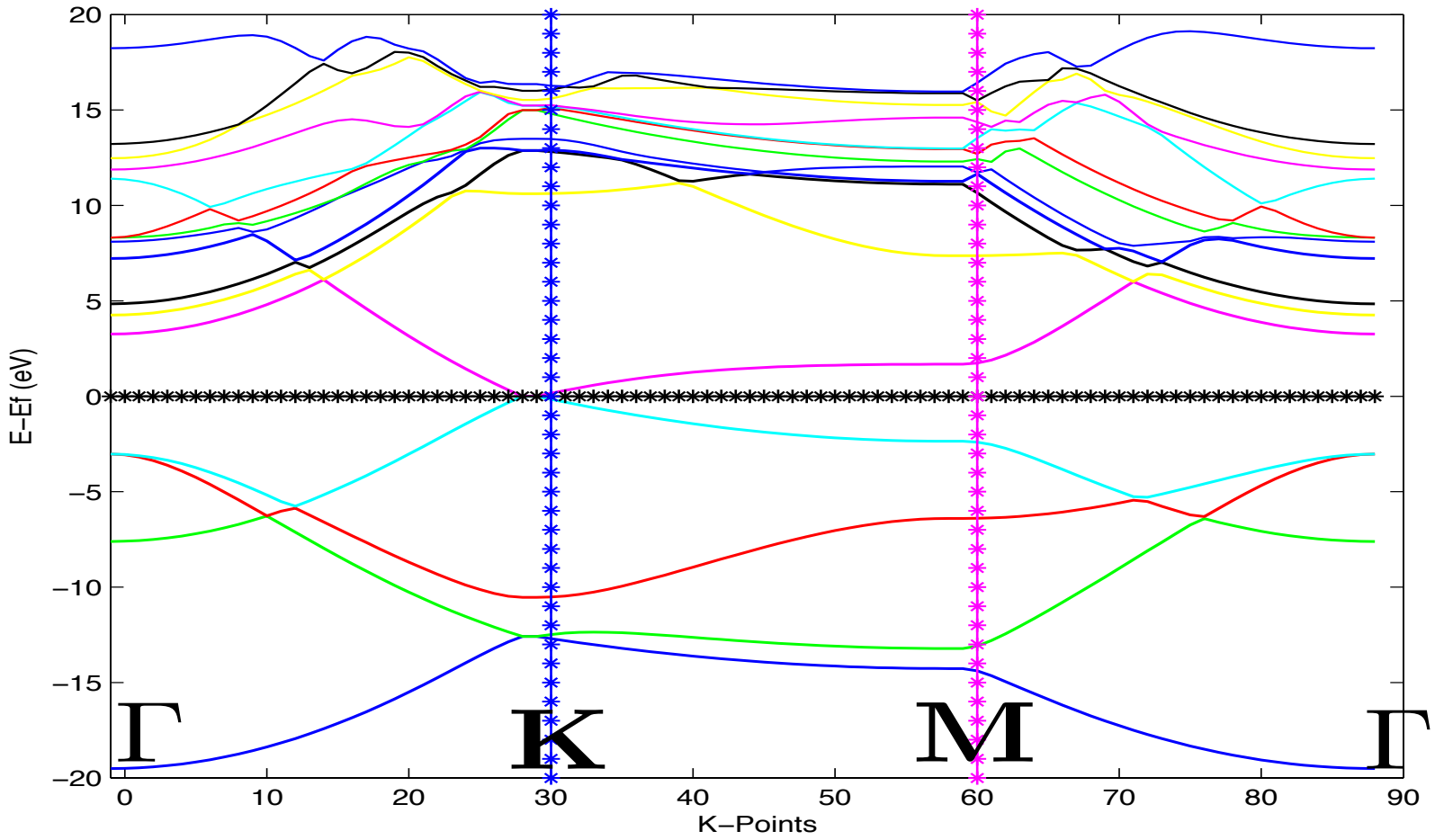


- Energy Set to Fermi Level

Band Structure Plot

Blochl-tetrahedron smearing

Spin Up



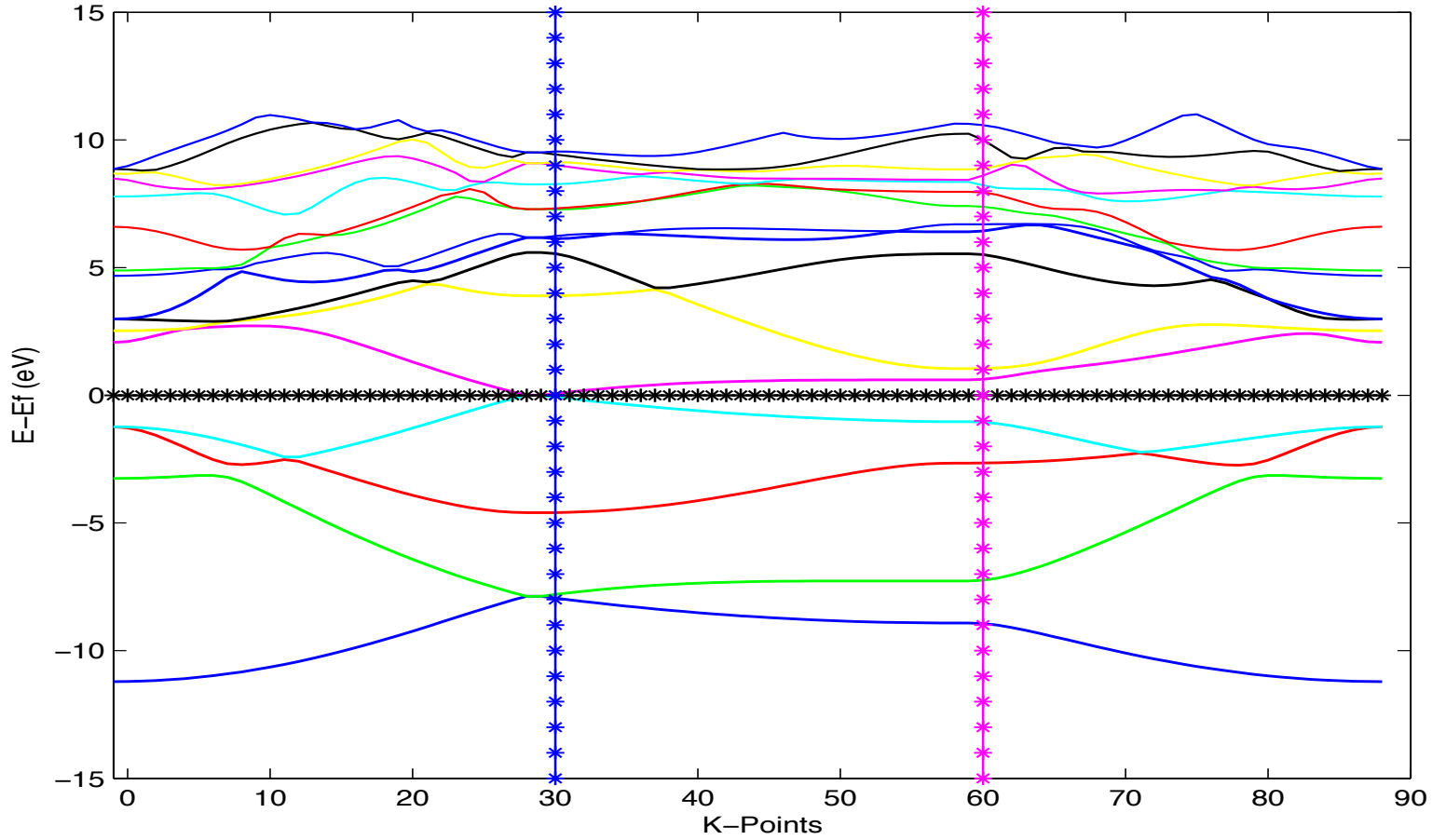
- Energy Set to Fermi Level

Silicene

Band Structure Plot

Blochl-tetrahedron smearing

Spin Up



- Energy Set to Fermi Level

Input files for SCF calculations for graphene

INCAR

```
SYSTEM = Graphene
PREC = Accurate
ISTART = 0
ICHARG= 2
ISPIN = 1
ENCUT = 500.0
ISIF = 2
IBRION = 1
NSW = 100
POTIM = .1
!NBANDS= 8
LREAL = .FALSE.
LWAVE = .TRUE.
ISMEAR = 0
LCHARG =.TRUE.
```

.FALSE.

KPOINTS

```
K-points
0
Gamma
12 12 1
0. 0. 0.
```

THANK YOU.