KATILARIN ELEKTRONİK YAPISININ BENZETİŞİMİ

Yoğun Madde Fiziğinde Kullanılan Yazılımlardan ab-initio Tekniği-1

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2.	**Yoğun Madde Fiziğinde Kullanılan Yazılımlardan ab-initio Tekniği**
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4.	Kristal Fiziği: Temel Kavramlar-2
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6.	Elektronik Bant Yapıları: İletkenlik durumları
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14.	FİNAL SINAVI

VASP (Vienna Simulation Method)

VASP Nedir?

VASP INPUTS

- POSCAR

- INCAR

- POTCAR

- KPOINTS

2D Bravais lattices

What is VASP?

The **V**ienna **A**b initio **S**imulation **P**ackage (VASP) is a computer program for atomic scale materials modelling, e.g. electronic structure calculations and quantum-mechanical molecular dynamics, from first principles.

VASP computes an approximate solution to the many-body Schrödinger equation, either within density functional theory (DFT), solving the Kohn-Sham equations, or within the Hartree-Fock (HF) approximation.

Hybrid functionals that mix the Hartree-Fock approach with density functional theory are implemented as well.

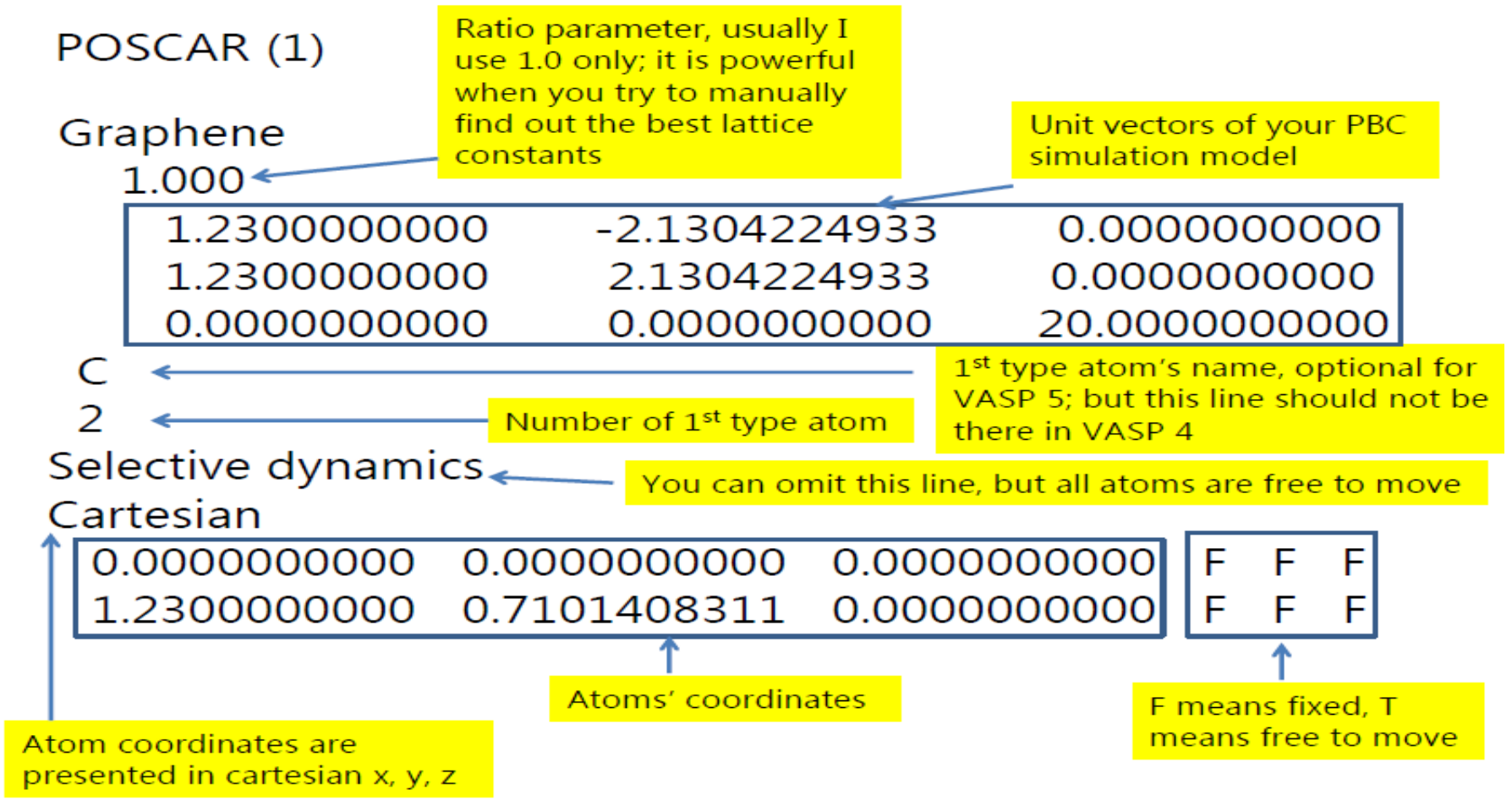
Furthermore, Green's functions methods (GW quasiparticles, and ACFDT-RPA) and many-body perturbation theory (2nd-order Møller-Plesset) are available in VASP.

VASP Input Files

http://cms.mpi.univie.ac.at/vasp/vasp/vasp.html

POSCAR	This file contains the lattice geometry and the ionic positions, optionally also starting velocities and predictor-corrector coordinates for a MD-run.
INCAR	It determines 'what to do and how to do it', and can contain a relatively large number of parameters. Most of these parameters have convenient defaults, and a user unaware of their meaning should not change any of the default values. Be very careful in dealing with the INCAR file, it is the main source of errors and false results
POTCAR	This file contains the pseudopotential for each atomic species used in the calculation. If the number of species is larger than one simply concats the POTCAR files of the species.
KPOINTS	The file KPOINTS must contain the k-point coordinates and weights or the mesh size for creating the k-point grid.

POSCAR


POSCAR (1)
Graphene
1.000
1.2300000000 -2.1304224933 0.0000000000
1.2300000000 2.1304224933 0.0000000000
0.0000000000 0.0000000000 20.0000000000
C
2
Selective dynamics
Cartesian
0.0000000000 0.0000000000 0.0000000000
1.2300000000 0.7101408311 0.0000000000
F F F
F F F
Ratio parameter, usually I use 1.0 only; it is powerful when you try to manually find out the best lattice constants
Unit vectors of your PBC simulation model
1st type atom's name, optional for VASP 5; but this line should not be there in VASP 4
Number of 1st type atom
You can omit this line, but all atoms are free to move
Atom coordinates are presented in cartesian x, y, z
Atoms' coordinates
F means fixed, T means free to move

POSCAR

POSCAR (2)

```
Graphene
  1.00000000000000
    1.2300000000000000   -2.1304224933000002    0.0000000000000000
    1.2300000000000000    2.1304224933000002    0.0000000000000000
    0.0000000000000000    0.0000000000000000   20.0000000000000000
  C
    2
Selective dynamics
Direct
  0.0000000000000000  0.0000000000000000  0.0000000000000000  F  F  F
  0.3333333333333357  0.6666666666666643  0.0000000000000000  F  F  F

 0.00000000E+00  0.00000000E+00  0.00000000E+00
 0.00000000E+00  0.00000000E+00  0.00000000E+00
```

Atom coordinates are presented in direct coordinates

velocities

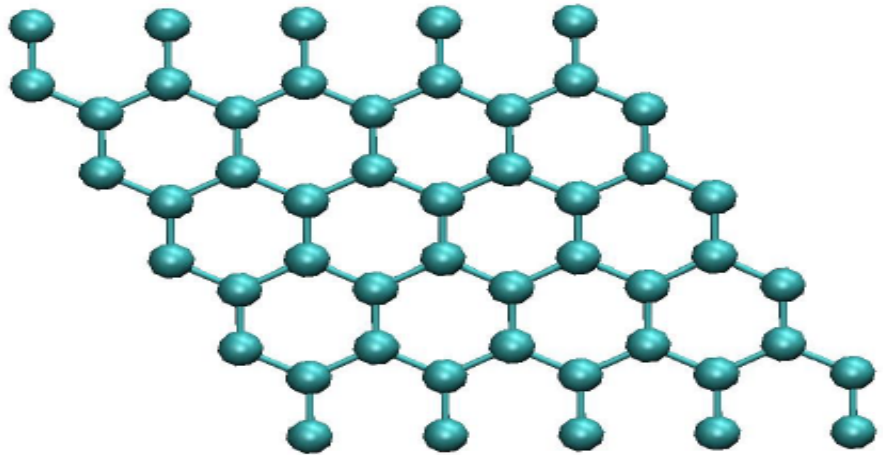
POSCAR

POSCAR (4) – How to visualize the simulation structure

1. By hand drawing
2. By imagination

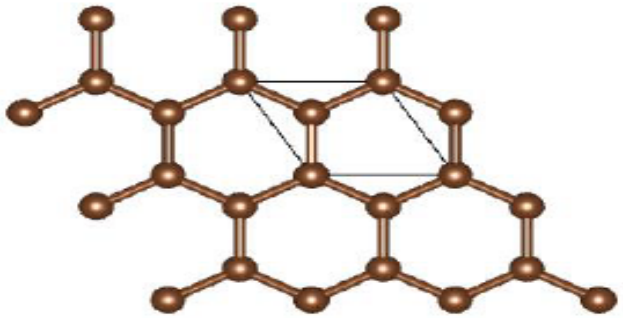
3. With the aid of some software

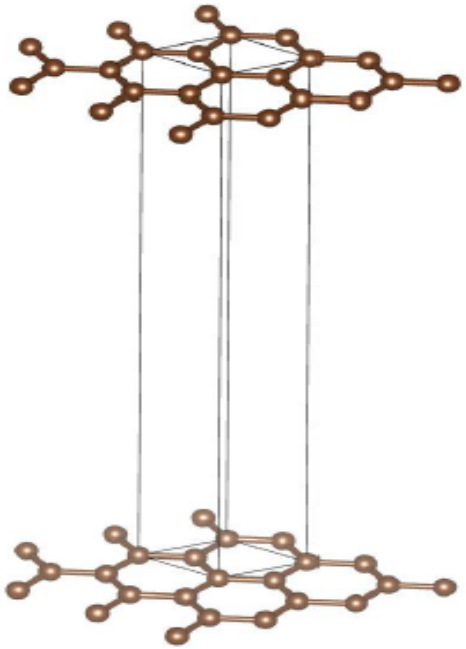
- VMD (Visual Molecular Dynamics) http://www.ks.uiuc.edu/Research/vmd/
- VESTA (Visualization for Electronic and Structural Analyisis http://jp-minerals.org/vesta/en/



POSCAR (4) – VESTA

1. Download VESTA and install it.
2. Download POSCAR or CONTCAR via Secure Shell or MobaXterm to some temp directory on your computer.
3. Open VMESTA and “file” -> “open” -> load CONTCAR
4. Click “Edit” -> “Bond…” - > “New”; Click “Object” -> “Boundary…” -> xmin = -1, ymin = -1





Primitive Unit Cell for Graphene

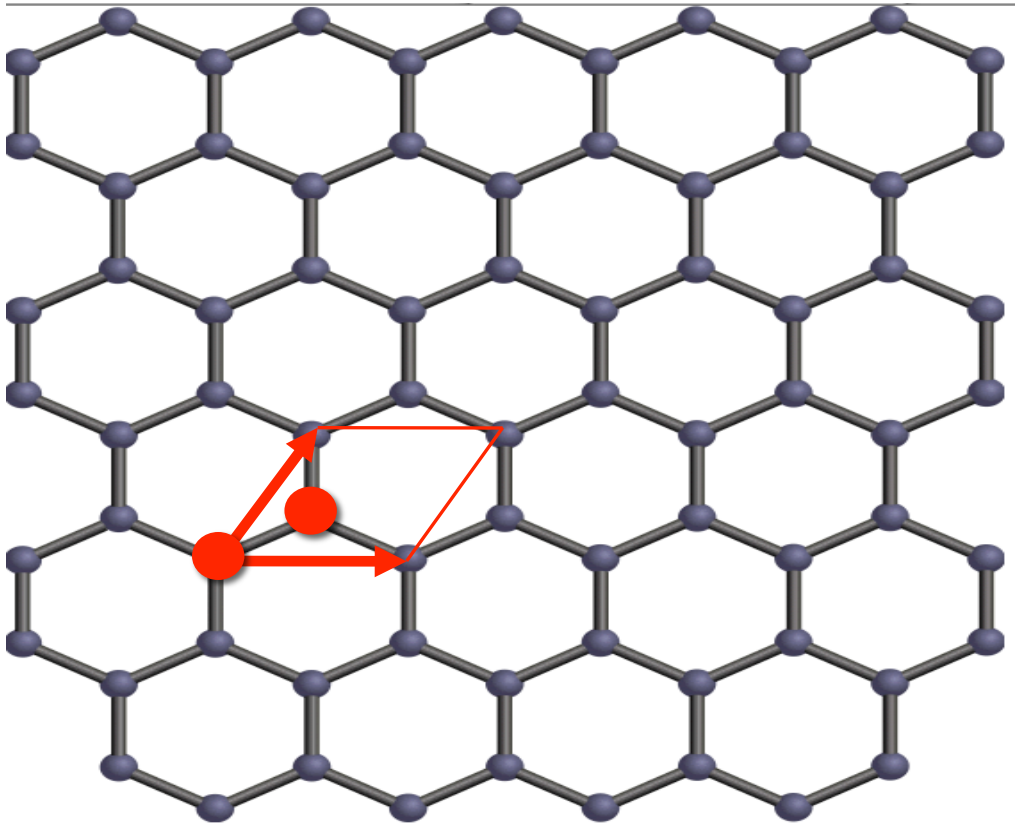
POSCAR

---------- Direct Tag ----------

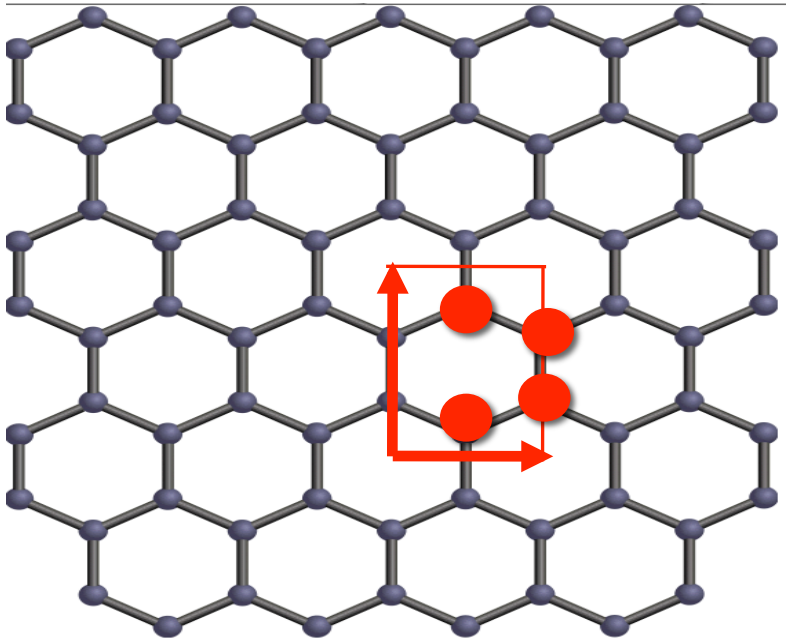
C
1.00000000000000
2.4670806653457333 0.0000000000000000 0.0000000000000000
1.2335403326728667 2.1365545293748203 0.0000000000000000
0.0000000000000000 0.0000000000000000 14.0000000000000000
C
2
Direct
0.3333333333333357 0.3333333333333357 0.5000000000000000
0.0000000000000000 0.0000000000000000 0.5000000000000000

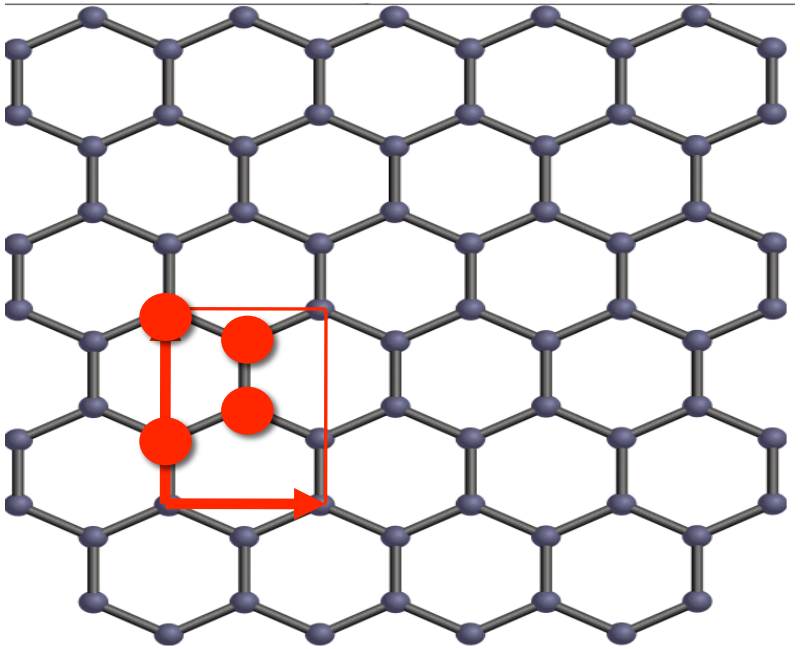
---------- CartesianTag ----------

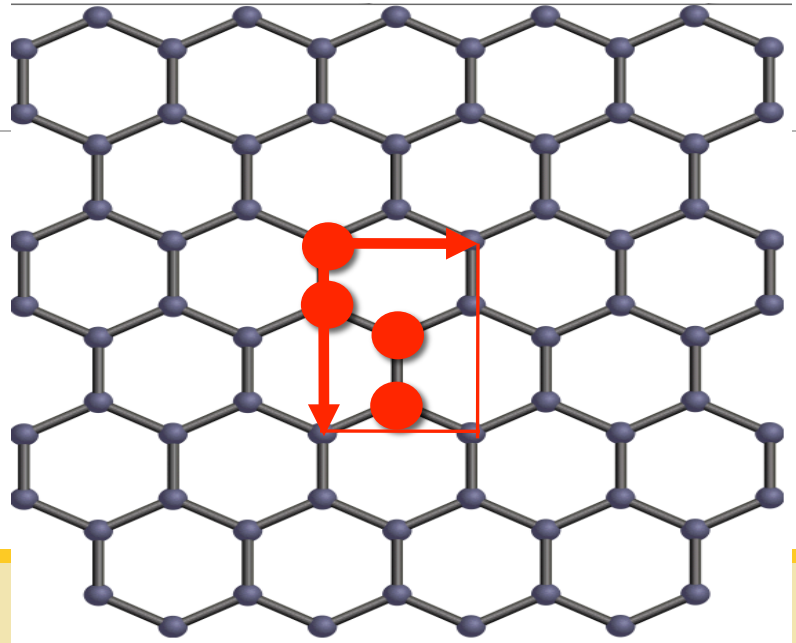
C
1.00000000000000
2.4670806653457333 0.0000000000000000 0.0000000000000000
1.2335403326728667 2.1365545293748203 0.0000000000000000
0.0000000000000000 0.0000000000000000 14.0000000000000000
C
2
Cartesian
1.2335400000000000 0.7121848000000000 7.0000000000000000
0.0000000000000000 0.0000000000000000 7.0000000000000000

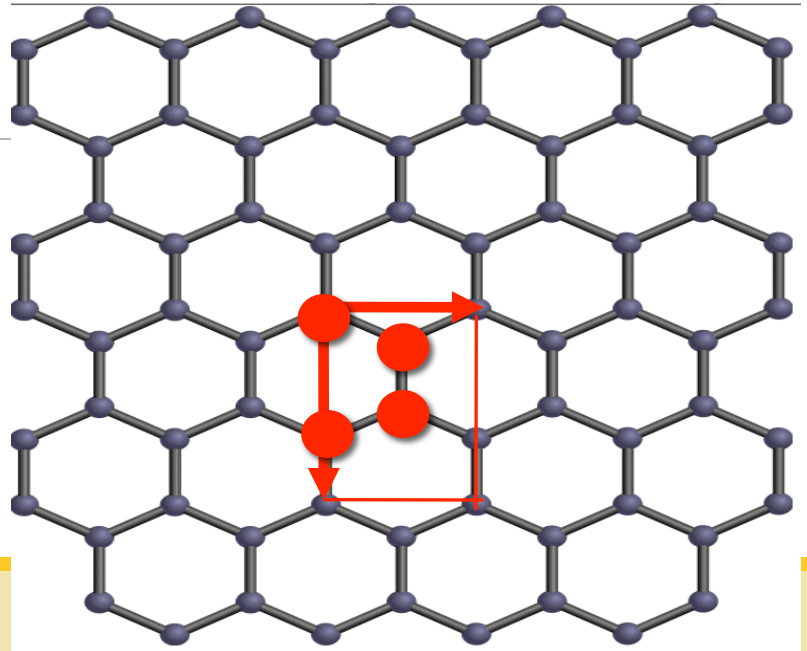


Orthogonal Unit Cell for Graphene









Orthogonal Unit Cell for Graphene

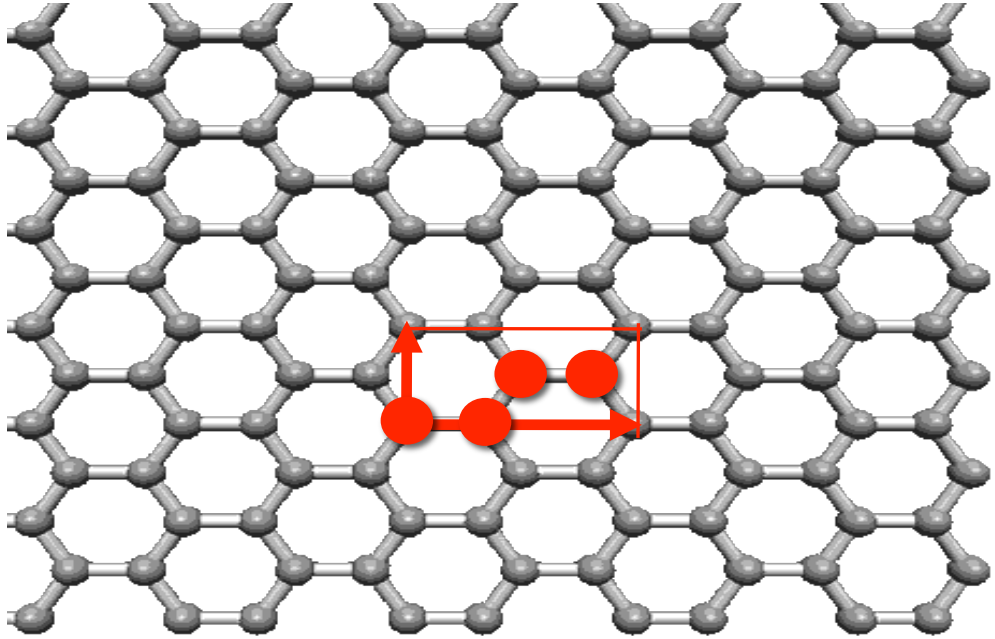
POSCAR

----------Cartesian Coordinate ----------

C
1.00000000
4.27500000 0.00000000 0.00000000
0.00000000 2.46817240 0.00000000
0.00000000 0.00000000 14.00000000
C
4
Cartesian
0.00000000 0.00000000 7.00000000
1.42500000 0.00000000 7.00000000
2.13750000 1.23408620 7.00000000
3.56250000 1.23408620 7.00000000

---------- Direct Coordinate ----------

C
1.00000000
4.27500000 0.00000000 0.00000000
0.00000000 2.46817240 0.00000000
0.00000000 0.00000000 14.00000000
C
4
Cartesian
0.00000000 0.00000000 0.50000000
0.33333333 0.00000000 0.50000000
0.50000000 0.50000000 0.50000000
0.83333333 0.50000000 0.50000000



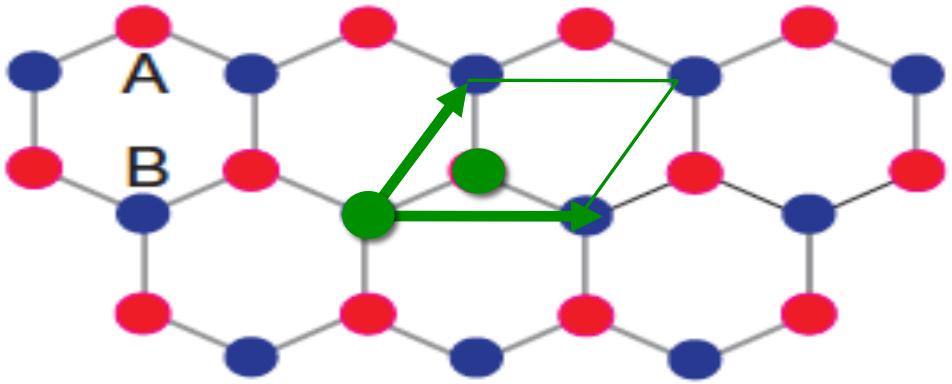
Primitive Unit Cell for Silicene

POSCAR

```
---------------------------------------- Direct Tag ----------------------------------
Si
   1.0000000000000000
     3.8600000000000000    0.0000000000000000    0.0000000000000000
     1.9300000000000000    3.3428580590000000    0.0000000000000000
     0.0000000000000000    0.0000000000000000   10.0000000000000000
   Si
   2
Direct
  0.0000000000000000  0.0000000000000000  0.5000000000000000
  0.3333330000000000  0.3333330000000000  0.5440000000000000

---------------------------------- CartesianTag ---------------------------------

Si
   1.0000000000000000
     3.8600000000000000    0.0000000000000000    0.0000000000000000
     1.9300000000000000    3.3428580590000000    0.0000000000000000
     0.0000000000000000    0.0000000000000000   10.0000000000000000
   Si
   2
Direct
  0.0000000000000000  0.0000000000000000  5.0000000000000000
  1.9300000000000000  1.1142849050000000  5.4400000000000000
```



Ezawa et al. New Journal of Physics ***14*** ***(2012) 033003***

INCAR

INCAR All list at http://cms.mpi.univie.ac.at/vasp/vasp/All_parameters_or_at_least_most.html

Important parameters

- ISTART = 0, 1, 2, or 3
- ICHARG = 0, 1, 2, 11, or 12
- ISYM = 0, 1, 2, or 3
- NELM = 60 or larger integer number
- EDIFF = 10^{-4} or some smaller number
- ENCUT = largest ENMAX or larger number
- ISPIN = 1, 2
- MAGMOM = specify the magnetization of each atom
- PREC = low, medium, high, nornal, accurate
- ISMEAR = -5, -4, -3, -2, 0, 1, 2 ..., 5
- SIGMA = 0.2 or smaller number
- NSW = some integer, the total ionic steps for configuration change
- EDIFFG = some small number (like 10^{-4} or -0.01)
- IBRION = -1, 0, 1, 2, 3, 5, 6, 7, 8
- POTIM = 0.5 or some number, size for atoms' moving
- ISIF = 0, 1, 2, 3, 4, 5, 6
- LWAVE = .F. or .T.
- LCHARG = .F. or .T.
- NPAR = some integer

INCAR

INCAR (1)

- ISTART = 0, 1, 2, or 3

  0: Start job: begin 'from scratch'. Initialize the orbitals according to the flag INIWAV (usually choose this one)

  1: restart with constant energy cut-off''. Continuation job -- read orbitals from file WAVECAR

  2: 'restart with constant basis set': Continuation job -- read orbitals from the file WAVECAR

  3: 'full restart including orbitals and charge prediction' ; Same as ISTART=2 but in addition a valid file TMPCAR must exist

- ICHARG = 0, 1, 2, 11, or 12

  0: Calculate charge density from initial orbitals. (WAVCAR)

  1: Read the charge density from file CHGCAR

  2: Take superposition of atomic charge densities (usually choose this one)

  11: To obtain the eigenvalues (for band structure plots) or the DOS for a given charge density read from CHGCAR.

  12: Non-selfconsistent calculations for a superposition of atomic charge densities.

INCAR

INCAR (2)

- ISYM = 0, 1, 2, or 3

  Switch symmetry on (ISYM=1, 2 or 3) or off (ISYM=0). For ISYM=2 a more efficient, memory conserving symmetrisation of the charge density is used. For ISYM=3, the forces and the stress tensor only are symmetrized, whereas the charge density is left unsymmetrized (VASP.5.1 only).

- NELM = 60 or larger integer number; too big (like 200) is already not OK for SC steps

  NELM gives the maximum number of electronic SC (self consistency) steps which may be performed.

- EDIFF = 10^{-4} or some smaller number

  Specifies the global break condition for the electronic SC-loop.

- ENCUT = largest ENMAX or larger number

  Cut-off energy for plane wave basis set in eV. All plane-waves with a kinetic energy smaller than ENCUT are included in the basis set: i.e.

$$\psi_{j,\mathbf{k}}(\mathbf{r}) = \sum_{\mathbf{G}} c_{j,\mathbf{k}+\mathbf{G}} e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}}. \qquad |\mathbf{G}+\mathbf{k}| < G_{\text{cut}} \quad \text{with} \quad E_{\text{cut}} = \frac{\hbar^2}{2m} G_{\text{cut}}^2$$

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INCAR

INCAR (3)

- ISPIN = 1, 2

  ISPIN=1 non spin polarized calculations are performed; ISPIN=2 spin polarized calculations are performed.

- MAGMOM = specify the magnetization of each atom

  Default: all atoms are assigned with magnetization 1.0 for ISPIN = 2

- PREC = low, medium, high, nornal, accurate

  Setting the detail number of plane waves expansion according to ENCUT and this tag.

- ISMEAR = -5, -4, -3, -2, 0, 1, 2 ..., 5

  Determines how the partial occupancies are set for each orbital; each number indicates one method.

- SIGMA = 0.2 or smaller number

  The smearing width parameter.

INCAR

INCAR (4)

- NSW = some integer, the total ionic steps for configuration change

  NSW sets the maximum number of ionic steps.

- EDIFFG = some small number (like 10^{-4} or -0.01)

  Optimization break criteria; positive: total energy difference, negative: force on each atom.

- IBRION = -1, 0, 1, 2, 3, 5, 6, 7, 8

  -1: fix all atoms; 0: molecular dynamics; 1: quasi-Newton (variable metric) algorithm optimization, 2: conjugate-gradient algorithm, 5~8: determine the Hessian matrix

- POTIM = 0.5 or some number, size for atoms' moving

- LWAVE = .F. or .T. (print out the WAVECAR (wave functions) or not)

- LCHARG = .F. or .T. (print out the CHGCAR (charge density) or not)

INCAR

INCAR (5)

- NPAR = some integer

  NPAR is set to 1. This implies distribution over plane wave coefficients only: all cores will work on every individual band, by distributing the plane wave coefficients over all cores. NPAR usually is set to be about the square root of the total cpu number. Then NPAR bands will run in MPI with NCORE/NPAR on one band.

- ISIF = 0, 1, 2, 3, 4, 5, 6

ISIF	calculate	calculate	relax	change	change
	force	stress tensor	ions	cell shape	cell volume
0	yes	no	yes	no	no
1	yes	trace only *	yes	no	no
2	yes	yes	yes	no	no
3	yes	yes	yes	yes	yes
4	yes	yes	yes	yes	no
5	yes	yes	no	yes	no
6	yes	yes	no	yes	yes
7	yes	yes	no	no	yes

THANK YOU.