VASP calculations of 2D Materials: Example of Silicon Carbide (2D-SiC)

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(1) Geometry Optimization (Lattice Relaxation)

(a) POSCAR:

```
SiC-PR
1.0
        2.5099000931          0.0000000000          0.0000000000
       -1.2549500465          2.1736372416          0.0000000000
        0.0000000000          0.0000000000         20.0000000000
    C   Si
    1    1
Direct
     0.666666687          0.333333343          0.500000000
     0.333333343          0.666666687          0.500000000
```

(b) KPOINTS:

```
Automatic mesh
0
Gamma
10 10 1
0  0  0
```

(c) INCAR:

```
#Global Parameters
  ISTART      = 1
  LREAL       = Auto
  PREC        = Normal
  LWAVE       = .TRUE.
  LCHARG      = .TRUE.
  ADDGRID     = .TRUE.

#Lattice Relaxation
  NSW         = 300
  ISMEAR      = 0
  SIGMA       = 0.05
  IBRION      = 2
  ISIF        = 3
```

```
  EDIFFG      = -1.5E-02
  PREC        = Accurate

# Parallelization
 LPLANE       = T
 NCORE        = 8
 LSCALU       = F
 NSIM         = 4
```

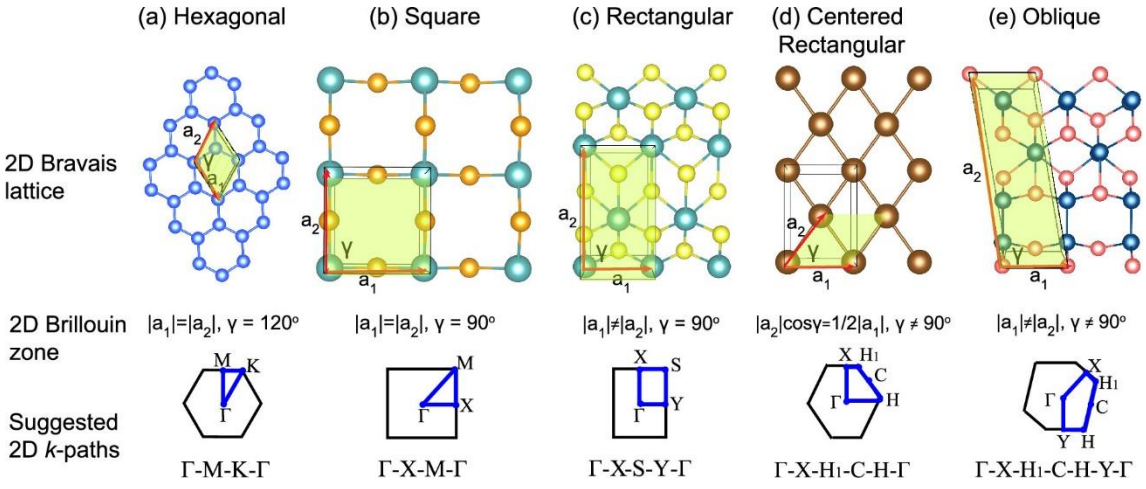
(d) POTCAR

Check here for selecting the correct pseudopotential file:
https://www.vasp.at/wiki/index.php/Available_PAW_potentials

(2) Band structure

To do band structure calculation, one need to prepare a primitive cell and corresponding K points path (K-path) alone Irreducible Brillouin Zone. Irreducible Brillouin Zone is the first Brillouin zone reduced by all of the symmetries in the points group of the lattice (point group of the crystal). Recognize and select high symmetry points, and link them along edges of Irreducible Brillouin Zone. This example will investigate the Band structure of 2D SiC without spin polarization without spin-orbital coupling

Details about the Brillouin zones for 2D materials can be found here:
J. Phys. Chem. Lett. 2022, 13, 50, 11581–11594 (https://doi.org/10.1021/acs.jpclett.2c02972)



In addition to the above information, there are other ways to find out the K-path automatically by using 1. pymatgen (https://pymatgen.org/)
2. seek-path (https://www.materialscloud.org/work/tools/seekpath)

At first, do geometry optimization, and then do a single-point self-consistent calculation to get the CHGCAR. The INCAR for that is given below.

```
Global Parameters
ISTART        = 1
LREAL         = Auto
PREC          = Normal
LWAVE         = .TRUE.
LCHARG        = .TRUE. # writes the CHGCAR file
ADDGRID       = .TRUE.

Lattice Relaxation
NSW           = 0 # for single point calculation
ISMEAR        = 0
SIGMA         = 0.05
IBRION        = 2
ISIF          = 3
EDIFFG        = -1.5E-02
PREC          = Accurate
```

The KPOINTS file for band and density of states calculation is given below. Always cross check this with the seek-path（https://www.materialscloud.org/work/tools/seekpath）

```
K-Path for 2D
20
Line-Mode
Reciprocal
0.0000000000   0.0000000000   0.0000000000     GAMMA
0.5000000000   0.0000000000   0.0000000000     M

0.5000000000   0.0000000000   0.0000000000     M
0.3333333333   0.3333333333   0.0000000000     K

0.3333333333   0.3333333333   0.0000000000     K
0.0000000000   0.0000000000   0.0000000000     GAMMA
```

Read the CHGCAR from single-point calculation and submit VASP band structure job.

```
##### initial I/O #####
SYSTEM        = SiC
ICHARG        = 11 #reads the CHGCAR file
LWAVE         = .TRUE.
LCHARG        = .TRUE.
```

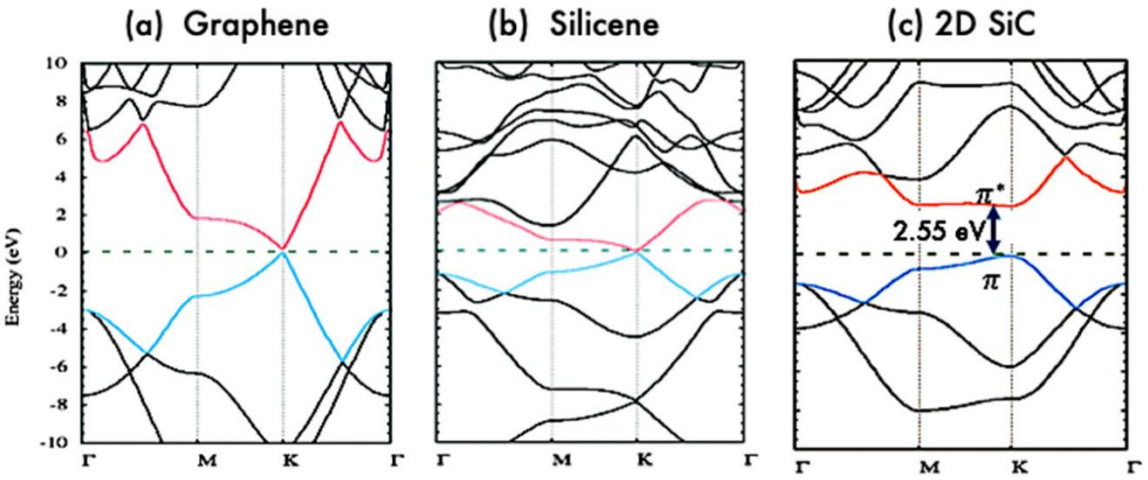
```
LVTOT          = .FALSE.
LVHAR          = .FALSE.
LELF           = .FALSE.
LORBIT         = 11
NEDOS          = 1000

##### SCF #####
ENCUT          = 500
ISMEAR         = 0
SIGMA          = 0.05
EDIFF          = 1E-6
NELMIN         = 5
NELM           = 300
GGA            = PE
LREAL          = .FALSE.
```

After calculation, do band structure post-processing. I would recommend to use a Python based utility, https://smtg-ucl.github.io/sumo/sumo-bandplot.html

Installation details can be found here: https://smtg-ucl.github.io/sumo/

Band structure can also obtain by pymatgen package

Check whether you're able to reproduce the band structure given below.



TASK: Try to generate the band structure of graphene and Silicene