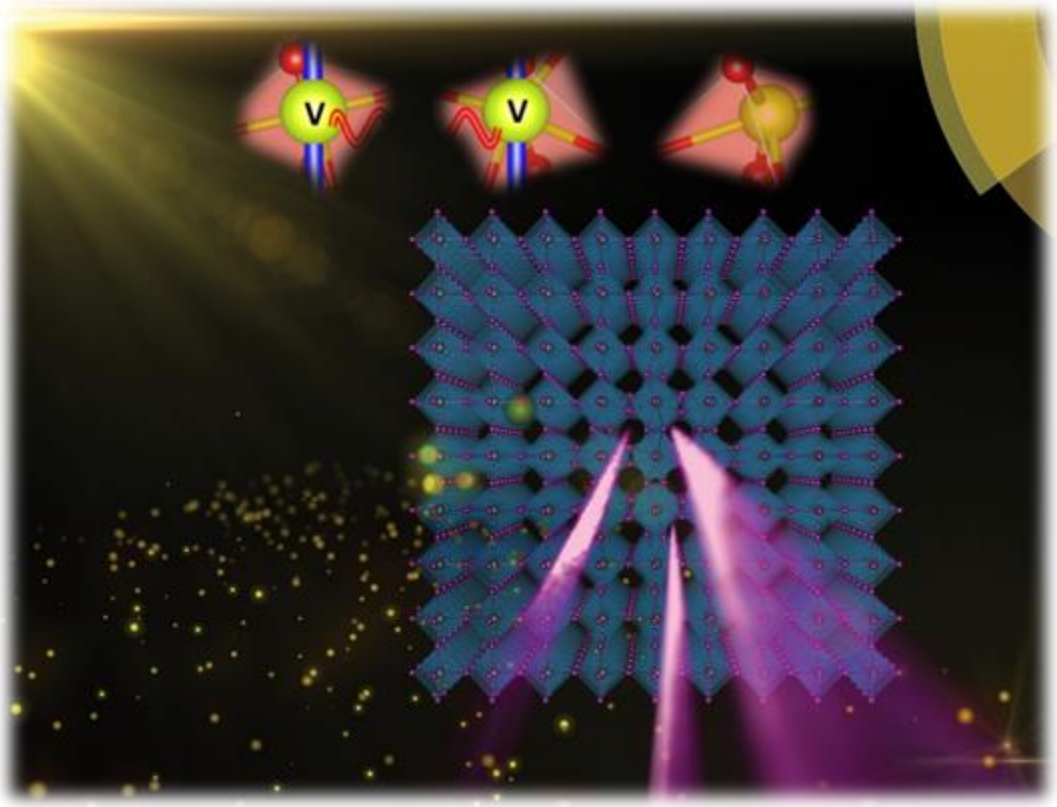
DFT Hands-on Graphene



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Prepare four input files

Download Graphene_files into desktop

Use WinScp to copy Graphene_files into Keldysh (XXX@keldysh.physics.udel.edu)

Go to work directory (XXX/graphene/primitive) using ssh
ssh XXX@keldysh.physics.udel.edu

Check files
primitive$ ls

```
[bkang@keldysh primitive]$ :/home/bkang/bootcamp/Graphene/primitive~>ls
 K6x6x1
[bkang@keldysh primitive]$ :/home/bkang/bootcamp/Graphene/primitive~>
```

K-mesh

Create 3 directories more.

primitive~>cp -r K6x6x1 K8x8x1

primitive~>cp -r K6x6x1 K10x10x1

primitive~>cp -r K6x6x1 K12x12x1

```
[bkang@keldysh primitive]$ :/home/bkang/bootcamp/Graphene/primitive~>ls
K10x10x1   K12x12x1   K6x6x1   K8x8x1
```

primitive~>nano K8x8x1/KPOINTS

```
k mesh
 0
Gamma
 6 6 1
 0  0  0
```

→

```
k mesh
 0
Gamma
 8 8 1
 0  0  0
```

← Change

Change K10x10x1/KPOINTS and K12x12x1/KPOINTS

Run four jobs

Primitive/K6x6x1~>./job.qs

Primitive/K8x8x1~>./job.qs

Primitive/K10x10x1~>./job.qs

Primitive/K12x12x1~>./job.qs

Compare total energy

primitive~>tail -n1 K6x6x1/OSZICAR K8x8x1/OSZICAR K10x10x1/OSZICAR K12x12x1/OSZICAR

```
==> K6x6x1/OSZICAR <==
   3 F= -.20123583E+02 E0= -.20108132E+02  d E =-.937694E-03


==> K8x8x1/OSZICAR <==
   3 F= -.20150310E+02 E0= -.20148738E+02  d E =-.125926E-02


==> K10x10x1/OSZICAR <==
   3 F= -.20155336E+02 E0= -.20154289E+02  d E =-.132833E-02


==> K12x12x1/OSZICAR <==
   3 F= -.20150807E+02 E0= -.20146556E+02  d E =-.124375E-02
```

Compare Geometries

primitive~>head -n15 K6x6x1/CONTCAR K8x8x1/CONTCAR K10x10x1/CONTCAR K12x12x1/CONTCAR

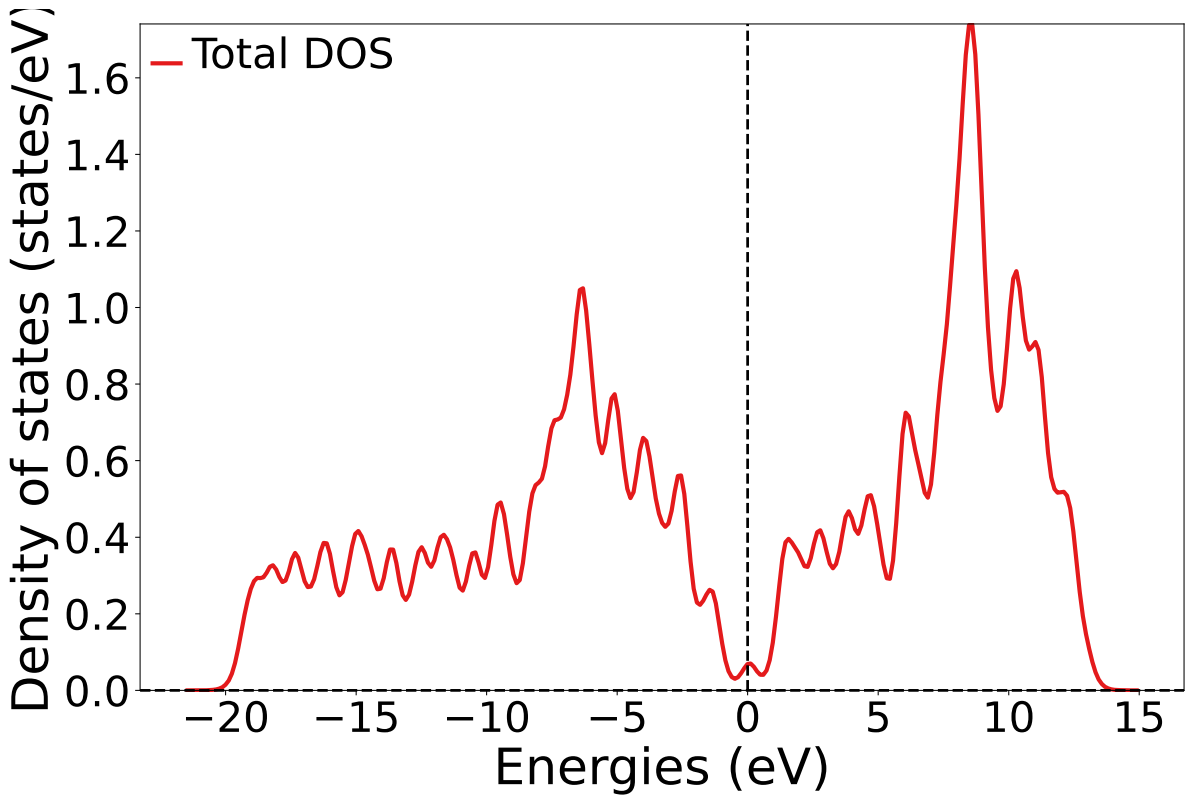
```
==> K6x6x1/CONTCAR <==
Graphene
   1.00000000000000
     1.2258535168902547   -2.1232405738909135    0.0000000000000000
     1.2258535168902547    2.1232405738909135   -0.0000000000000000
     0.0000000000000000   -0.0000000000000000    8.0411210144034850
   C
     2
Selective dynamics
Direct
  0.6666666666666714  0.3333333333333286  0.0000000000000000   T   T   F
  0.3333333333333286  0.6666666666666714 -0.0000000000000000   T   T   F

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


==> K8x8x1/CONTCAR <==
Graphene
   1.00000000000000
     1.2253556416867477   -2.1223782287426110   -0.0000000000000000
     1.2253556416867477    2.1223782287426110    0.0000000000000000
     0.0000000000000000    0.0000000000000000    8.0476567301625970
   C
     2
Selective dynamics
Direct
  0.6666666666666714  0.3333333333333286  0.0000000000000000   T   T   F
  0.3333333333333286  0.6666666666666714 -0.0000000000000000   T   T   F

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


==> K10x10x1/CONTCAR <==
Graphene
   1.00000000000000
```

Plot density of states

Transfer K12x12x1/vasprun.xml on Keldysh to /Graphene_files/dos_plot on Desktop

C:…/Graphene_files/dos_plot> python dos_tot.py

Open “dos.pdf”



Band structure

Download Graphene_files into desktop

May skip

Use WinScp to copy Graphene_files into Keldysh (XXX@keldysh.physics.udel.edu)

Go to work directory (XXX/graphene/band) using ssh

ssh XXX@keldysh.physics.udel.edu

Check files

band$ ls

```
[bkang@keldysh band]$ :/home/bkang/bootcamp/Graphene/band~>ls
INCAR  INCAR_band  job.qs  KPOINTS  KPOINTS_band  POSCAR  POTCAR
```

View files

INCAR

```
SYSTEM = graphene
ISMEAR = -1
SIGMA = 0.2
```

KPOINTS

```
k mesh
 0
Gamma
 12 12 1
 0  0  0
```

POSCAR

```
Graphene
   1.00000000000000
     1.225378101371026   -2.122417130056902    0.000000000000000
     1.225378101371026    2.122417130056902    0.000000000000000
     0.000000000000000    0.000000000000000    8.047361725424558
   C
     2
Selective dynamics
Direct
  0.666666666666714  0.333333333333286  0.000000000000000   T   T   F
  0.333333333333286  0.666666666666714 -0.000000000000000   T   T   F
```

Prepare CHGCAR: Run job

band$ ./job.qs

```
DAV:  13    -0.201177157432E+02   -0.29748E-04   -0.68023E-06   344   0.226E-02
   1 F= -.20117716E+02 E0= -.20113465E+02  d E =-.850246E-02
 writing wavefunctions
```

band$ ll

```
[bkang@keldysh band]$ :/home/bkang/bootcamp/Graphene/band~>ll
total 2796
-rw-rw-r-- 1 bkang bkang 348760 Aug 14 10:04 CHG
-rw-rw-r-- 1 bkang bkang 525510 Aug 14 10:04 CHGCAR
-rw-rw-r-- 1 bkang bkang    555 Aug 14 10:04 CONTCAR
-rw-rw-r-- 1 bkang bkang  11073 Aug 14 10:04 DOSCAR
-rw-rw-r-- 1 bkang bkang   6406 Aug 14 10:04 EIGENVAL
-rw-rw-r-- 1 bkang bkang   1482 Aug 14 10:04 IBZKPT
-rw-r--r-- 1 bkang bkang     44 Aug 14 09:56 INCAR
-rw-r--r-- 1 bkang bkang     87 Aug 14 09:57 INCAR_band
-rwxr-xr-x 1 bkang bkang     77 Aug 14 09:56 job.qs
-rw-r--r-- 1 bkang bkang     34 Aug 14 09:56 KPOINTS
-rw-r--r-- 1 bkang bkang    723 Aug 14 09:57 KPOINTS_band
```

Prepare band_run directory

```
band$ mkdir band_run
band$ cp * band_run
band$ cd band_run
```

Prepare input files in band_run directory

```
band_run$ cp CONTCAR POSCAR
band_run$ cp INCAR_band INCAR
band_run$ cp KPOINTS_band KPOINTS
```

View files in band_run directory

INCAR

```
SYSTEM = graphene

ICHARG = 11 #charge read file
ISMEAR = 0; SIGMA = 0.1;
LORBIT = 11
```

POSCAR

KPOINTS

```
HEX (hexagonal) G-M-K-G-A-L-H-A L-M K-H
128   ! 128 grids
Line-mode
reciprocal
   0.0000   0.0000   0.0000   ! \Gamma
   0.5000   0.0000   0.0000   ! M
   0.5000   0.0000   0.0000   ! M
   0.3333   0.3333   0.0000   ! K
   0.3333   0.3333   0.0000   ! K
   0.0000   0.0000   0.0000   ! \Gamma
   0.0000   0.0000   0.0000   ! \Gamma
   0.0000   0.0000   0.5000   ! A
   0.0000   0.0000   0.5000   ! A
   0.5000   0.0000   0.5000   ! L
   0.5000   0.0000   0.5000   ! L
   0.3333   0.3333   0.5000   ! H
   0.3333   0.3333   0.5000   ! H
   0.0000   0.0000   0.5000   ! A
   0.5000   0.0000   0.5000   ! L
   0.5000   0.0000   0.0000   ! M
   0.3333   0.3333   0.0000   ! K
   0.3333   0.3333   0.5000   ! H
```

Run job

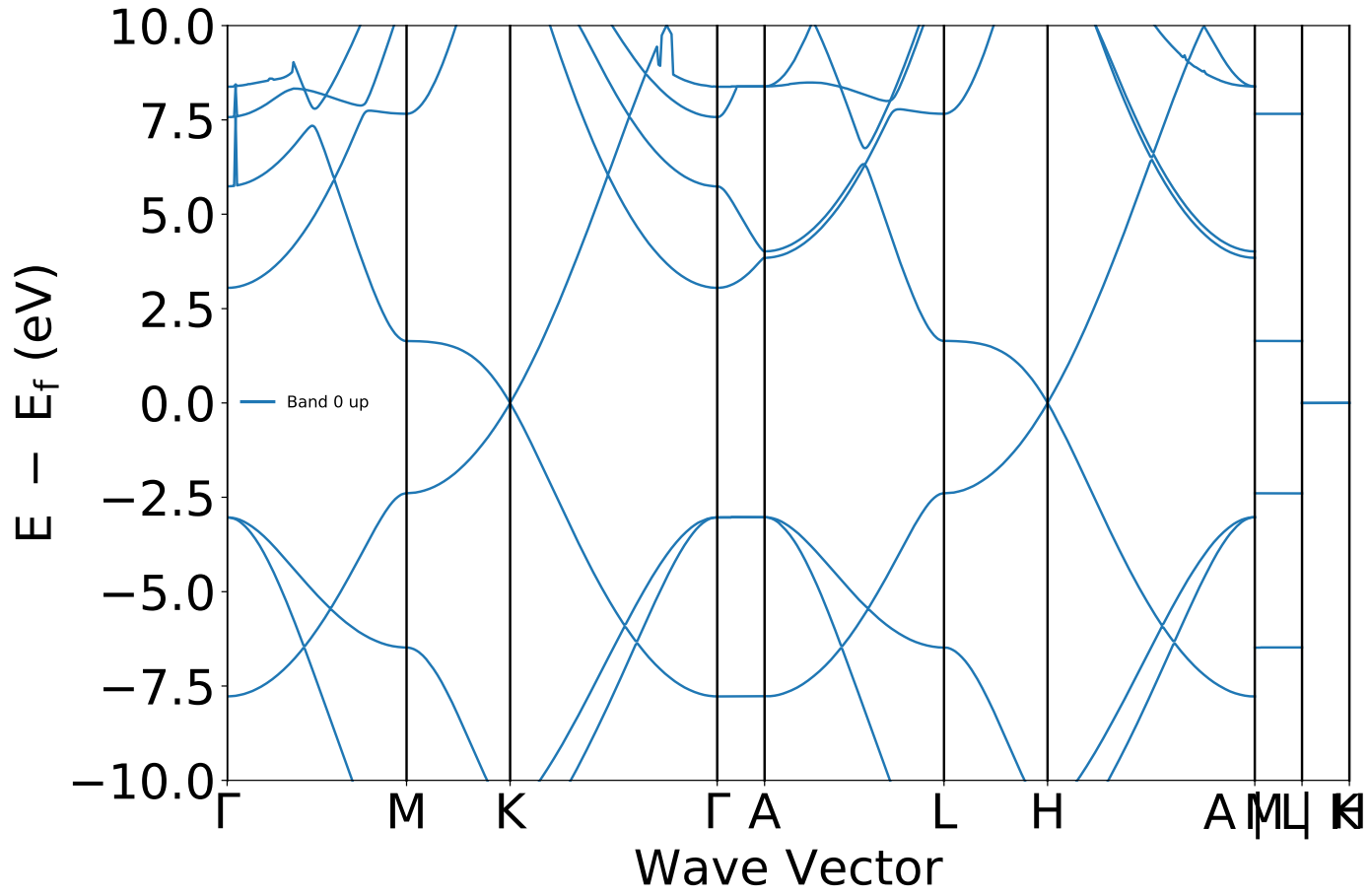
band_run$ ./job.qs

Plot band structure

Transfer band_run/vasprun.xml, KPOINTS, POSCAR on Keldysh
to /Graphene_files/band_plot on Desktop

C:…/Graphene_files/band_plot> python band.py

Open “band.pdf”

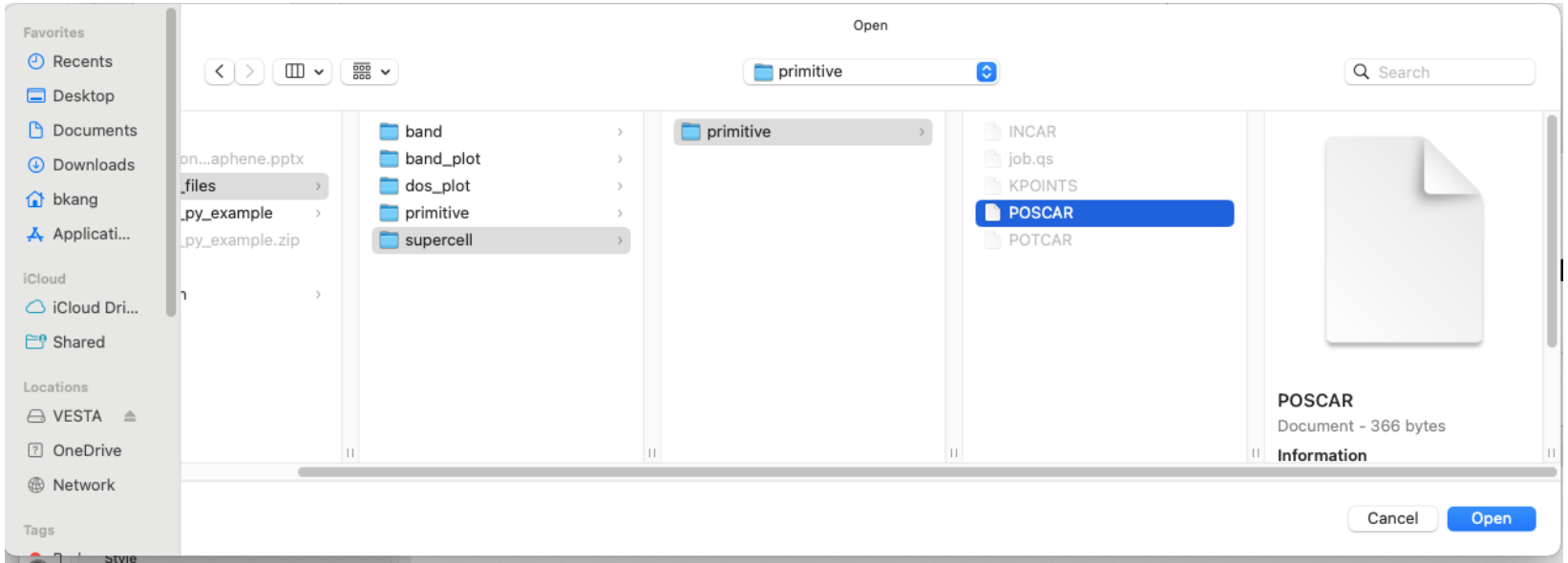


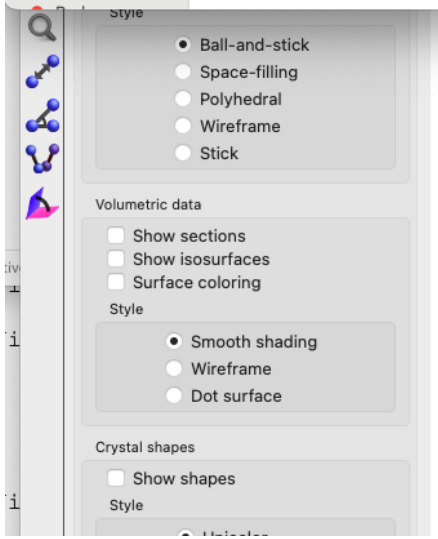
Supercell

Go to work directory C:XXX/Graphene_files/supercell/primitive on Desktop

Open POSCAR using Vesta

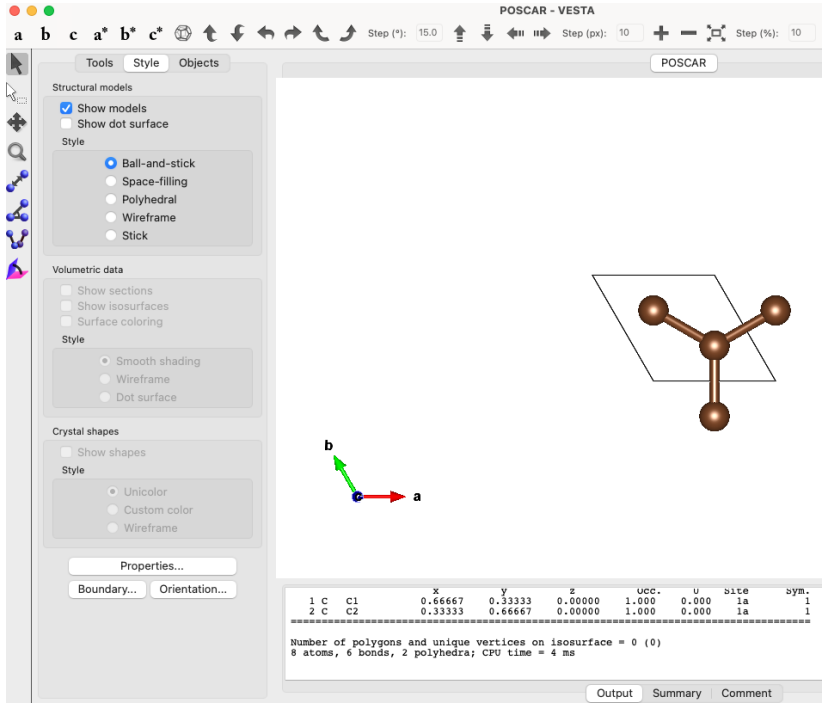
C:XXX/Graphene_files/supercell/primitive/POSCAR on Desktop



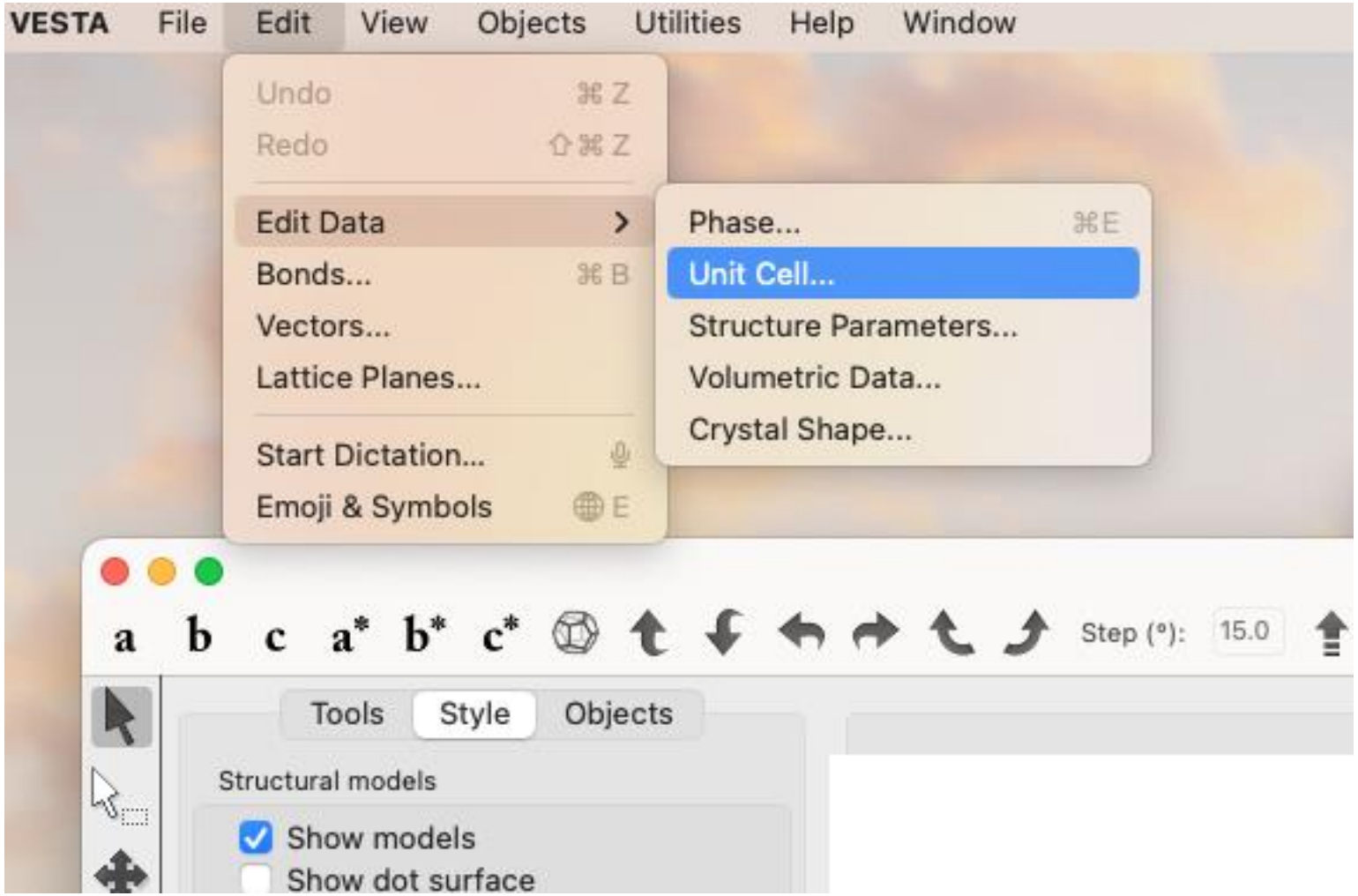


VESTA

Visualization for Electronic and STructural Analysis

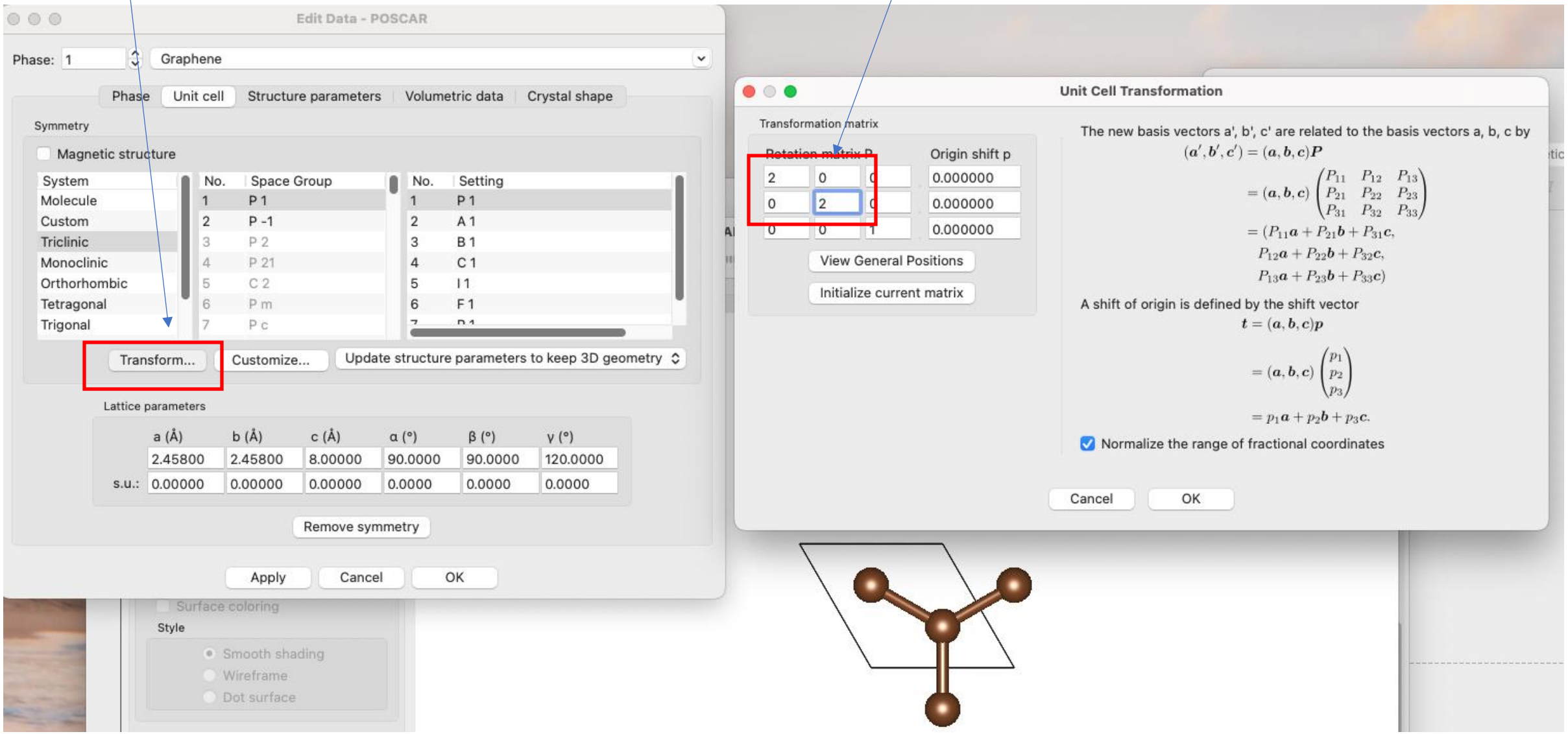


Select Unit Cell menu



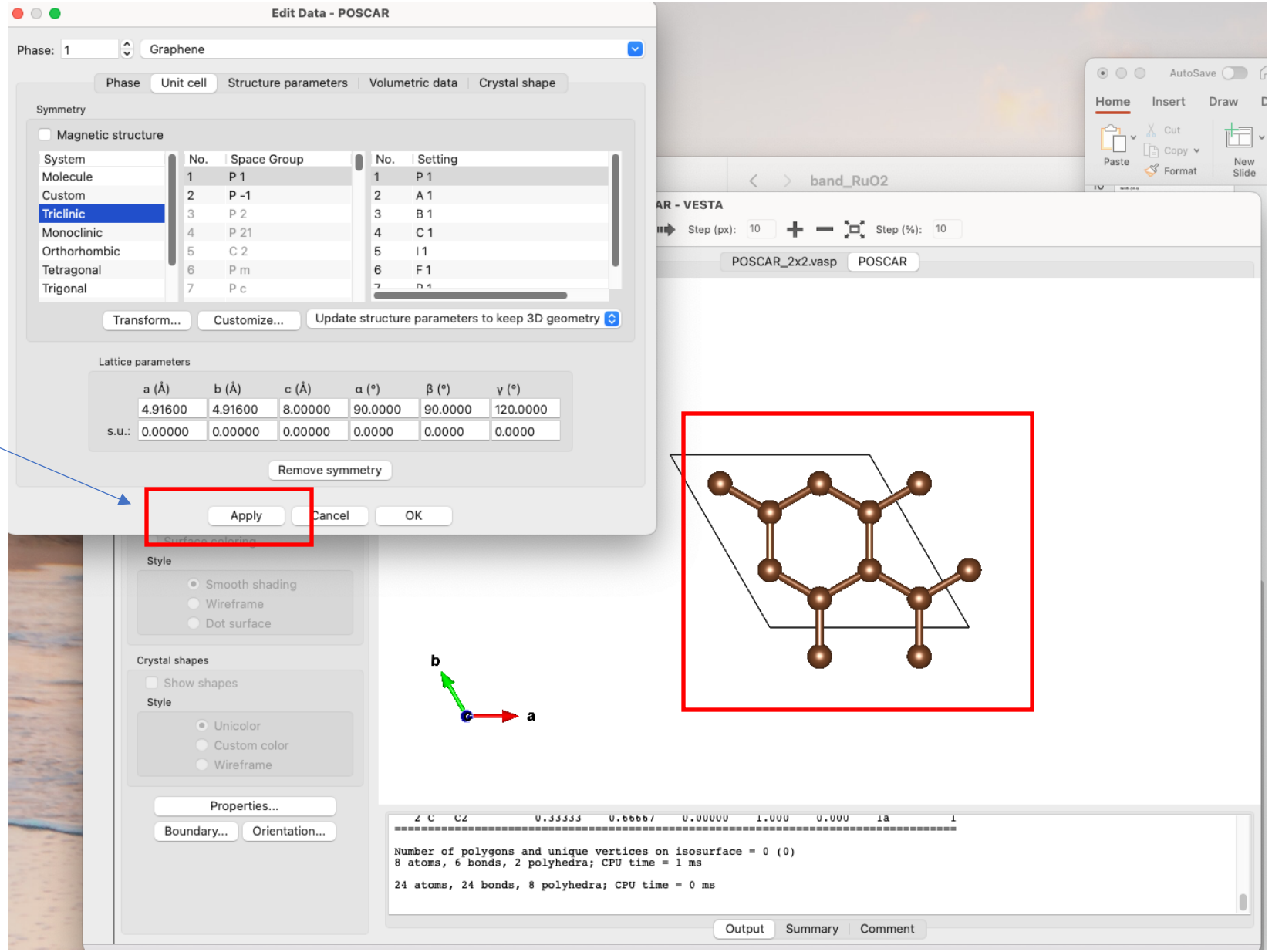
Click

Change from 1 to 2

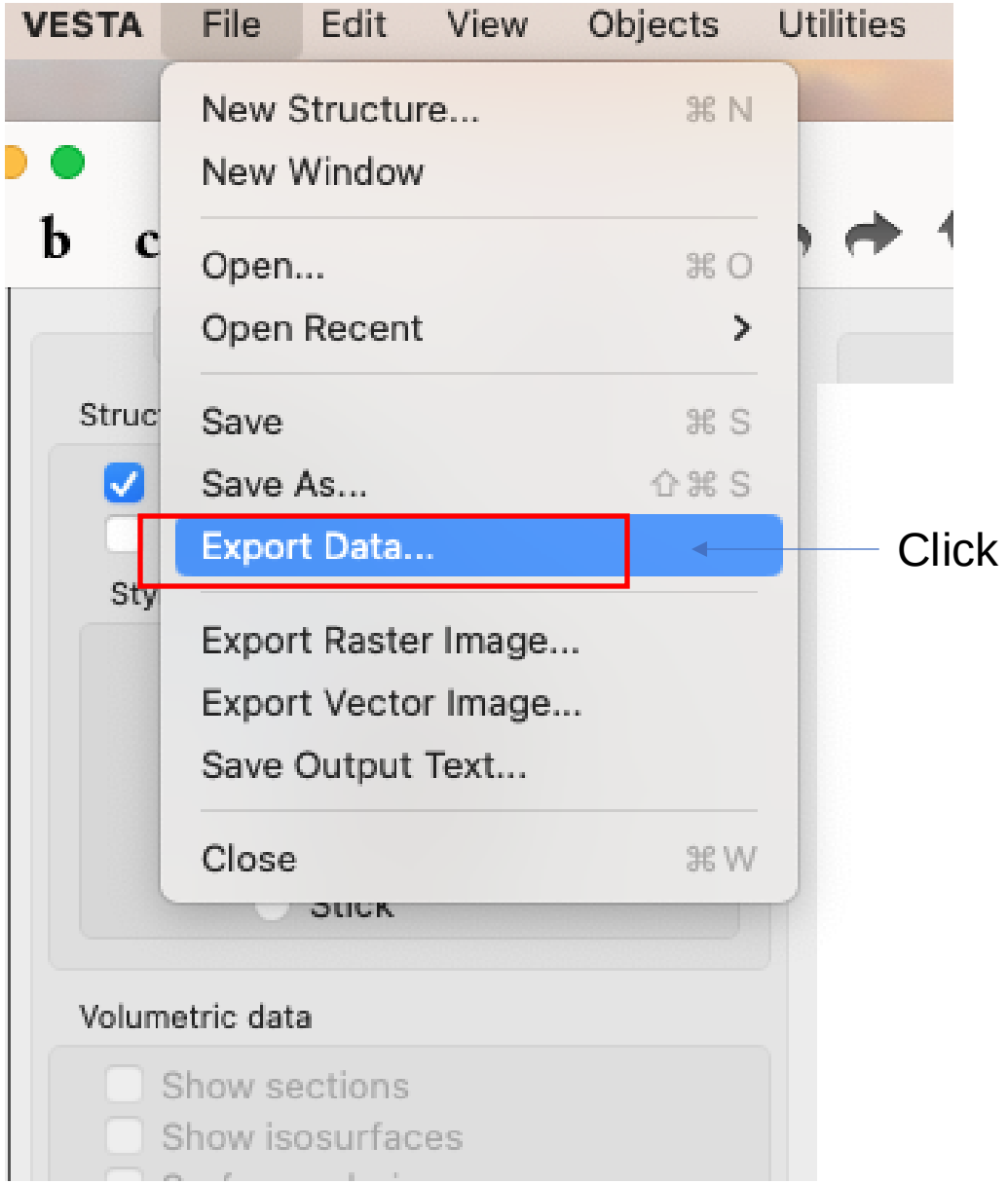


Click Ok, yes, apply, ok

Click

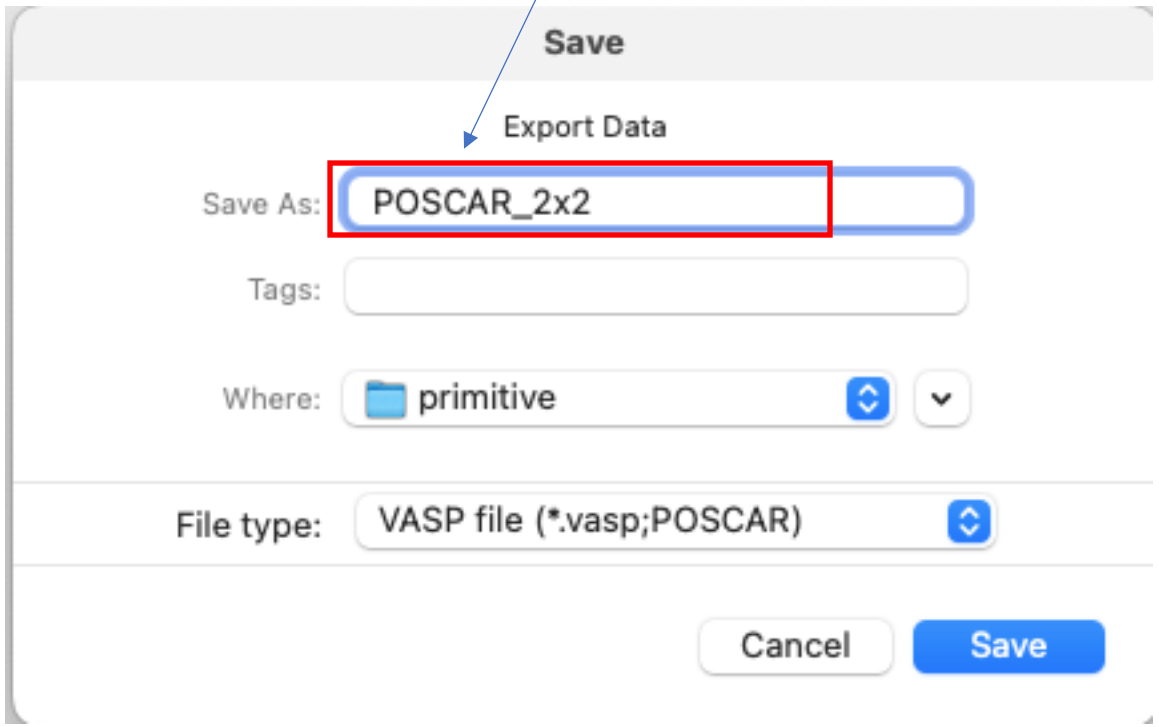


Export 2x2x1 supercell



Click

Type name



Check POSCAR_2x2.vasp

```
Graphene
1.0
        4.9159998894        0.0000000000        0.0000000000
       -2.4580005116        4.2573804619        0.0000000000
        0.0000000000        0.0000000000        8.0000000000
   C
   8
Direct
    0.333333343         0.166666672         0.000000000
    0.333333343         0.666666687         0.000000000
    0.833333373         0.166666672         0.000000000
    0.833333373         0.666666687         0.000000000
    0.166666672         0.333333343         0.000000000
    0.166666672         0.833333373         0.000000000
    0.666666687         0.333333343         0.000000000
    0.666666687         0.833333373         0.000000000
```

Tasks

Create directory with POSCAR (from POSCAR_2x2.vasp)

Create directory with POSCAR (from POSCAR_3x3.vasp)

Create directory with POSCAR (from POSCAR_4x4.vasp)

Transfer the directories to Keldysh

Run jobs

Plot density of states

Calculate energy per atom

Thank you