1. VASP calculation on small molecule

a) The results are shown in Table 1.

Table 1. The H-O distance and H-O-H angle before and after relaxation.

	H-O distance (Å)	**H-O-H angle (°)**
Before relaxation	0.95471	104.8628
After relaxation	0.97242	104.5215

b) The internal energy as a function of ENCUT is shown in Fig. 1. According to the official guide, the plane-wave-basis set only includes the plane waves that have a kinetic energy smaller than ENCUT. If the ENCUT value is set too low, the plane wave basis set will be insufficient to accurately describe the electronic wavefunctions. As the value of ENCUT is increased, the calculation of the total energy becomes more accurate, and converges to a stable value. It's essential to ensure that calculations are performed at or above this converged ENCUT value to obtain accurate results. It's worth noting that while increasing ENCUT improves accuracy, it also increases the computational cost of the simulation. Hence, it's a common practice to perform convergence tests: increasing ENCUT in steps until the energy stabilizes, thus ensuring accuracy without unnecessary computational expense.

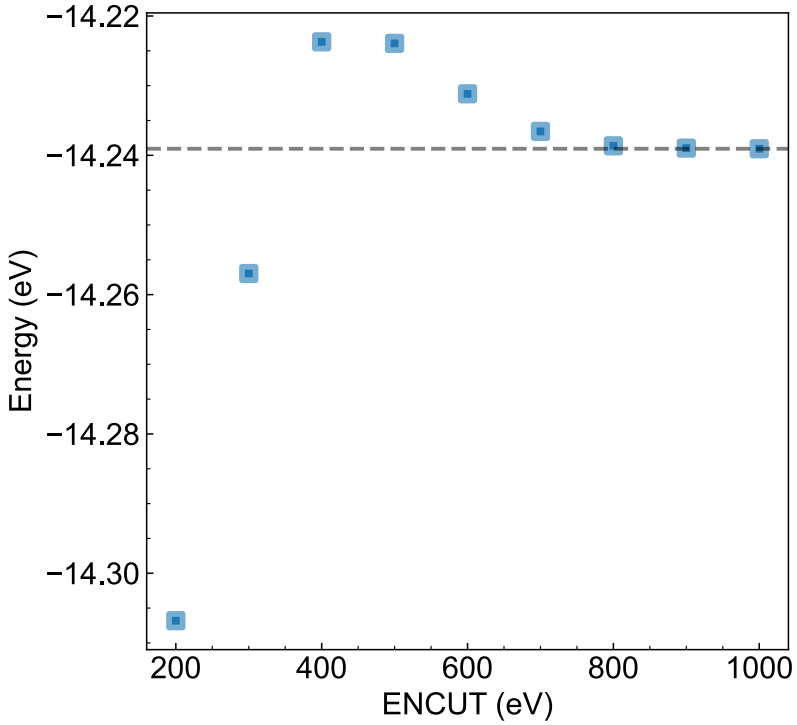

Figure 1. The convergence of Energy with respect to ENCUT.

2. VASP calculation on condensed matter

a) The reproduced plot is shown in Fig. 2.

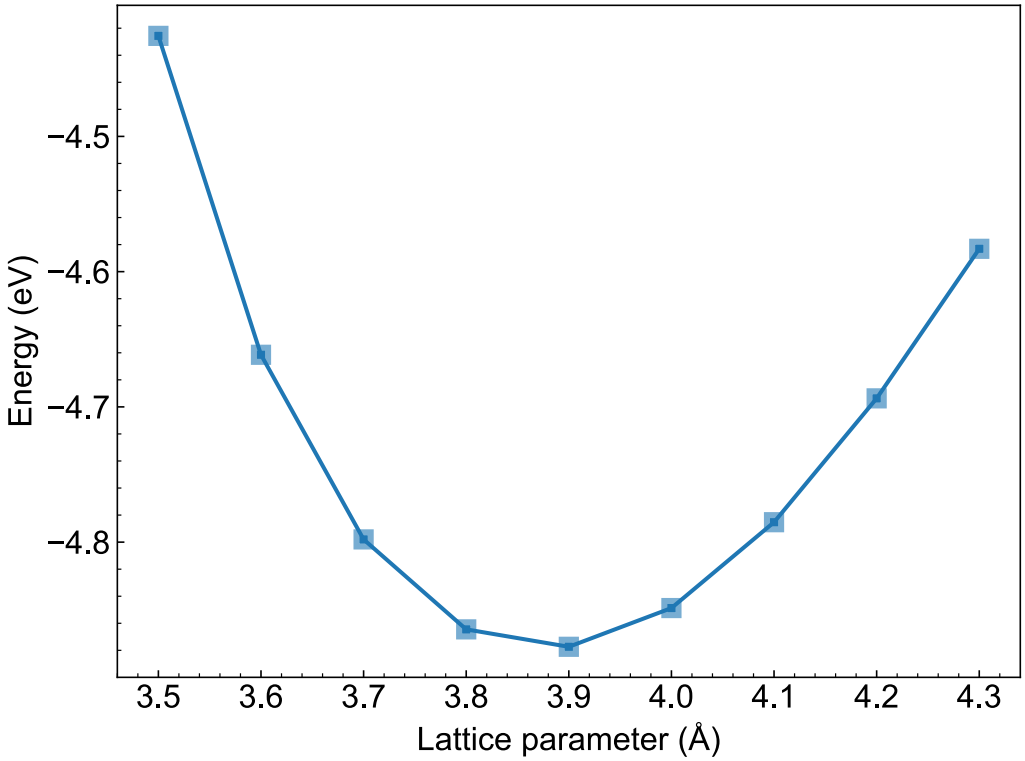

Figure 1. The energy of fcc Si as a function of lattice parameter.

b) In order to find the lattice parameter with lowest energy using one simulation, I choose to do a ionic relaxation using conjugate gradient algorithm by setting `IBRION = 2` in the INCAR file. According to the official guide, the parameter ISIF determines which principal degrees-of-freedom are allowed to change in relaxation and molecular dynamics runs. In this problem, we do not want to change the fcc crystal structure of Si but only want to determine the cell parameter with the lowest energy. Therefore, we need to set both the positions and the cell shape to be unchanged but change the cell volume. This corresponds to an ISIF value of 7. The modified INCAR file is as follows:

```
System = fcc Si
ISTART = 0
ICHARG = 2
ENCUT  = 240
ISMEAR = 0
SIGMA  = 0.1
NSW    = 20
IBRION = 2
ISIF   = 7
EDIFF  = -0.0001
```

The lattice parameter I found is 3.86629 Å, which is very close to the minimum point in Fig. 1.

3. LAMMPS simulation

I choose the simulation of granular pouring and chute flow. The movie (movie.mp4) and LAMMPS log file (log.lammps) can be found in the folder named LAMMPS_simulation.