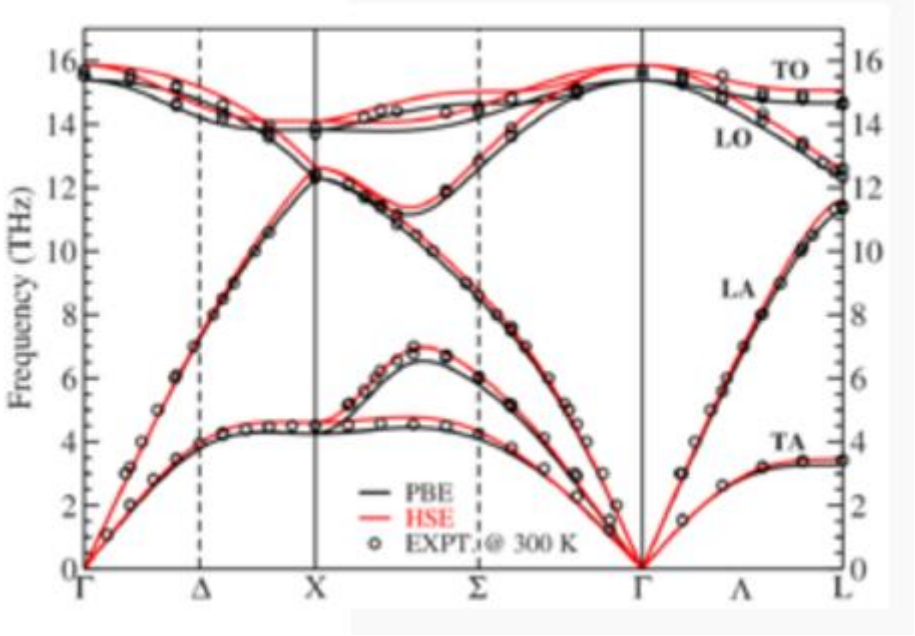
The Γ-phonon in silicon

In short, the task is: calculate the frequency of the phonon(s) at the Γ-point in crystalline silicon.

That should be sufficient to get started. If you don't see how to tackle this, you can go to the next page for more hints. But give it a thought first without looking at the hint. It would be nice if you can solve this alone.

From this picture you can see what your answer should be – this allows to verify your result:



Technical settings: this pseudopotential, ecutwfc=40 Ry, ecutrho=160 Ry and a 10x10x10 k-mesh guarantee you a fair precision. Calculations take less than 30 seconds per case.

Further hints in case you get stuck:

Start with a primitive unit cell for silicon (you can do it with a conventional cell too, which has 4x more atoms – it will just take you a bit more calculation time). The primitive cell has two atoms. That's indeed a crystal with a basis, which means we have acoustic as well as optical phonons. At Γ, there are only optical phonons. Optical phonons at Γ correspond to atoms that oscillate in the unit cell only, such that their overall center of mass does not move.

Displace the two atoms in the primitive unit cell in opposite directions (does in matter in which directions? The phonon band structure on the preceding page holds a clue for that). Calculate the total energy. Repeat this for a few positive as well as negative displacement around the equilibrium positions. Plot the total energy as a function of the displacement (distance). Fit a parabola through these data, and use its fitted curvature to determine the frequency. Be careful with the units. Compare your frequency with what you see in the preceding picture.