

Quiz-4 ASESMA – 2010
THERE WILL BE THREE PRIZES AT THE ENED OF THE SCHOOL
THIS QUIZ WILL COUNT IN DETERMINING WHO GETS THE PRIZES

NAME:

INSTITUTION:

Select all the correct answers. There may be more than one correct answer per question.

1. When is an ionic relaxation complete:
 - Xa. When all forces are zero (within some tolerance)
 - b. When the sum of forces is zero (within some tolerance)
 - Xc. When the energy stops changing (within some tolerance)

The sum of forces should always be zero whether the system is in equilibrium or not.

2. A crystal has 3 electrons per cell. Is it expected to be a metal or insulator?
 - Xa. Metal
 - b. Insulator
 - c. This is not enough information to determine whether it is metal or insulator.An odd number of electrons mean at least one partially filled band.
3. In PWSCF should you increase the cutoff for the charge density above the default value when you:
 - a. Calculate the energy for a metal
 - b. Relax a structure
 - Xc. Use an ultrasoft pseudopotentialIt is a general rule for all codes that the charge density is more rapidly varying for an ultrasoft pseudopotential, due to the added function in the ultrasoft pseudopotential. This means higher Fourier components in the density, and that means increasing the cutoff for the charge density above the factor of 4 that is sufficient for norm-conserved potentials. The fact that the default value is always 4 applies only to PWSCF.
4. In magnetic systems
 - Xa. The number of up and down spins is different.
 - b. The Fermi energy for up and down spins is different.
 - Xc. The density of states (DOS) is differentUp and down spins are always different in magnetic systems – different bands, number, and DOS. But the Fermi energy is the same for all electrons.
5. Suppose you run calculations with a functional that allows up and down spins, for example, the local spin density (LSD) functional.
 - a. The result is always spin polarized.
 - Xb. The result may or may not be polarized.
 - Xc. This is the way one can find whether or not the lowest energy state is spin polarized or not.If you start from a polarized state it will relax to zero polarization if the system is non-magnetic, e.g., in Si. The LSD is the same as the LDA if there is no polarization.
6. In which case do you expect a LO-TO splitting of optic phonons at the zone center ($k=0$), that is, a splitting due electric fields

- a. Al (fcc)
- Xb. AlAs (zinc blende)
- c. Si (diamond)

Only for an ionic insulator will the phonon have a net electric field (called the macroscopic electric field).

7. There is much work to find better exchange-correlation functionals.
 - a. The total energy calculated for a crystal always decreases if the exchange-correlation functional is improved
 - b. The lattice constant is always in better agreement with experiment
 - Xc. One hopes the lattice constant and other properties are improved but that must be tested for every different type of material

When you try to improve the functional there is no guarantee that anything will improve. Even if one thing is improved there is no guarantee that anything else will improve. Finally, no approximation works for everything!

8. Which k-point mesh would you need to calculate the energy of an isolated H₂O molecule:
 - a. A 4x4x4 unshifted
 - b. A 4x4x4 shifted
 - Xc. The Gamma point (k=0) only
 - d. A Gamma-X-L-Gamma path

If the molecules are isolated, every k-point should give the same answer. Only one point is needed

9. The phonon and electron bands have the same Brillouin Zone
 - Xa. True
 - b False

All waves have the same BZ in a crystal.

10. Which of the following does NOT change if a supercell is increased in volume, for example, if one compares a calculation for Si in the 2 atoms primitive cell with a calculation for a cube with 8 atoms in the cell
 - a. The total energy for the cell
 - Xb. The energy per atom
 - Xc. The force on an atom
 - Xd. The gap between the highest occupied band and the lowest empty band

The energy per atom, the force on an atom and the gap are all well-defined quantities that can be measured experimentally They should not depend on what cell you use. The energy per cell is proportional to the number of atoms in the cell, so it changes.

11. Compared to the local density approximation (LDA) a calculation with a generalized gradient approximation (GGA)
 - Xa. Tends to have lower total energy (more negative)
 - b. Does not change the energy but it may change the forces
 - Xc. Both energy and forces change

Everything changes! It is generally lower because that added term is negative.

12. A MgSiO₃ crystal has 20 atoms per primitive cell. How many phonons bands does it have?
 - Xa. 60
 - b. 3
 - c. 5

There are always $3N$ phonon bands for a 3 dimensional crystal (also called phonon dispersion curves or phonon branches or phonon modes)

13. For the same crystal, how many acoustic bands does it have?

- a. 60
- Xb. 3
- c. 5

There are always 3 acoustic modes for a 3 dimensional crystal; they are the phonon bands that have frequency proportional to k for small k . They are often called “modes” since they represent the three velocities of sound for small k (long wavelength).

14. For which type of problem do you expect to need a higher energy cutoff for the number of plane waves?

Xa. As a rule a higher cutoff is needed for calculation of energy than for calculation of stress

b. As a rule a lower cutoff is needed for calculation of energy than for calculation of stress

c. There no general rule.

The stress depends upon the cutoff more due to “Pulay terms” This is rather technical, but you should realize that this is what actually happened in the computer calculations you did.