

Carbon, silicon, germanium and tin all adopt the diamond structure. Diamond has a band gap of 5.5 eV, while silicon absorbs wavelengths shorter than 1100 nm. Predict the band gaps of germanium and tin.

**Tin is a metal. It is a conductor with no band gap.**

**The longest wavelength,  $\lambda$ , absorbed by silicon is 1100 nm. This corresponds to the *minimum* energy required to excite an electron: the band gap. The energy,  $E$ , is related to  $\lambda$  through Planck's equation  $E = hc / \lambda$ .**

**The band gap in silicon is therefore:**

$$E = hc / \lambda = (6.626 \times 10^{-34} \text{ J s}) \times (2.998 \times 10^8 \text{ m s}^{-1}) / (1100 \times 10^{-9} \text{ m}) \\ = 1.8 \times 10^{-19} \text{ J}$$

**As 1 eV =  $1.602 \times 10^{-19}$  J, this corresponds to:**

$$E = (1.8 \times 10^{-19} / 1.602 \times 10^{-19}) \text{ eV} = 1.1 \text{ eV}$$

**The band gap decreases down the group: 5.5 eV (C), 1.1 eV (Si) and 0 eV (Sn). The band gap in germanium will be between that for Si and Sn, around the average of 0 and 1.1 eV.**

Predict the band gap of SiC, which also has a diamond like structure, but with Si bonded to 4 C atoms, and C bonded to 4 Si atoms.

**It will be around an average of the values for C and Si:**

$$\text{predicted band gap} = \frac{1}{2} (5.5 + 1.1) \text{ eV} = 3.3 \text{ eV}$$

Use the information in the following table to predict the density of tin.

Element	Atomic Mass	Density ( $\text{g cm}^{-3}$ )	Bond length (pm)
Ge	72.64	5.323	244
Sn	118.7		280.

**Density depends on the mass and the volume:**

$$\text{density} = \text{mass} / \text{volume}$$

**The volume of a crystal will increase as the cube of the bond length:**

$$\text{volume of tin} = (280 / 244)^3 \times \text{volume of germanium}$$

**The mass will increase as the atomic mass increases:**

$$\text{mass of tin} = (118.7 / 72.64) \times \text{mass of germanium}$$

**As the density of germanium is  $5.323 \text{ g cm}^{-3}$ , the density of tin will therefore be:**

$$\text{density of tin} = \text{density of germanium} \times (118.7 / 72.64) / (280 / 244)^3 \\ = 5.323 \text{ g cm}^{-3} \times (118.7 / 72.64) / (280 / 244)^3 = 5.76 \text{ g cm}^{-3}$$

Answer:  $5.76 \text{ g cm}^{-3}$

**Marks**  
**2**

- In the spaces provided, explain the meaning of the following terms. You may use an example, equation or diagram where appropriate.

(a) covalent bond

**A covalent bond describes the situation where an aggregation of 2 or more atoms is stabilised by the delocalisation of electrons among these atoms**

(b) electronegativity

**A measure of the tendency of an atom to attract electrons within a covalent bond.**

(c) free radical

**An atom or molecule with one or more unpaired electrons.**

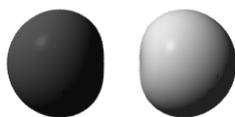
(d) band gap

**The energy gap between the top of the valence band and the bottom of the conductance bands (the HOMO-LUMO gap) in a solid.**

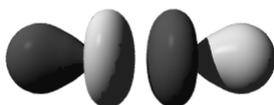
- In the spaces provided, explain the meaning of the following terms. You may use an example, equation or diagram where appropriate.

(a) antibonding molecular orbital

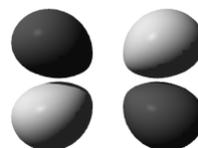
**An orbital with a nodal plane perpendicular to the bond. Occupation of an antibonding orbital lowers the bond order and weakens a bond. The diagram below show the antibonding orbitals produced from overlap of s-orbitals ( $\sigma^*$  - A) and p-orbitals ( $\sigma^*$  - B and  $\pi^*$  - C):**



$\sigma^*$  - A



$\sigma^*$  - B



$\pi^*$  - C

(b) emission spectroscopy

**The study of radiation emitted as an atom or molecule relaxes from an initial excited state. Because of the quantized nature of energy levels, emission occurs at particular wavelengths which are characteristic of the atom or molecule.**

(c) band gap

**The energy gap between the valence and conductance bands in a solid. The diagram below shows this schematically.**

**When this gap is large (as opposite), the solid is an insulator as there is insufficient energy to excite an electron from the filled valence band to the empty conductance band.**



**When this gap is small (as opposite), the solid is a semi-conductor as, except at very low temperatures, there is thermal excitation into the conductance band.**



(d) a triple bond

**A "bond" between two atoms involving the sharing of three electron pairs. It usually consists of 1  $\sigma$ -bond and 2  $\pi$ -bonds. The most common molecules containing triple bonds are  $N_2$  and CO. Triple bonds are represented by drawing three lines between the atoms. For example,  $N \equiv N$  and  $C \equiv O$ .**

- In the spaces provided, explain the meaning of the following terms. You may use an example, equation or diagram where appropriate.

(a) diamagnetic

**A description of an atom or molecule with no unpaired electron spins and hence no net magnetic moment.**

(b) covalent bond

**A low energy arrangement of two or more atoms arising from the delocalisation of electrons in molecular orbitals.**

(c) Hund's rule

**The requirement that degenerate orbitals are all half-filled with electrons with parallel spins before any of the degenerate orbitals is filled.**

(d) electrical conductor

**A material in which charged groups can flow in response to an applied electric field or potential. In the case where the material is a solid and the charged "groups" are electrons, this requires a small to zero band gap.**

- In the spaces provided, explain the meaning of the following terms. You may use an example, equation or diagram where appropriate.

(a) Pauli exclusion principle

**The principle that states that no two electrons in an atom or molecule can have the same set of quantum numbers. It limits the number of electrons that can occupy an orbital to two.**

(b) electronegativity

**The ability of an atom to attract electron density towards itself in a covalent bond. Fluorine is the most electronegative element.**

(c) ionic bond

**The low energy state found in ionic solids associated with the Coulombic attraction of unlike charged ions.**

(d) paramagnetic

**A property of an atom, ion, molecule or solid resulting from the presence of at least one unpaired electron spin. Paramagnets are attracted towards a magnetic field.**

(e) n-type semiconductor

**A semiconductor has electrical conductivity in between that of a metal and that of an insulator. A n-type semiconductor is obtained by adding a type of atoms to a semiconductor in order to increase the number of negative charge carrier. For example, doping a group 14 element such as Si with a group 15 element such as As leads to extra electrons in the conductance band which are free to move and carry the charge.**

(e)  $\sigma$  bond

**A bond produced by the occupation of a  $\sigma$ -bonding molecular orbital. This orbital is made by overlap of atomic orbitals, such as end-on/end-on overlap of p-orbitals or of s-orbitals, to produce a molecular orbital with no nodes along the internuclear axis. The electron density is along the internuclear axis.**

--

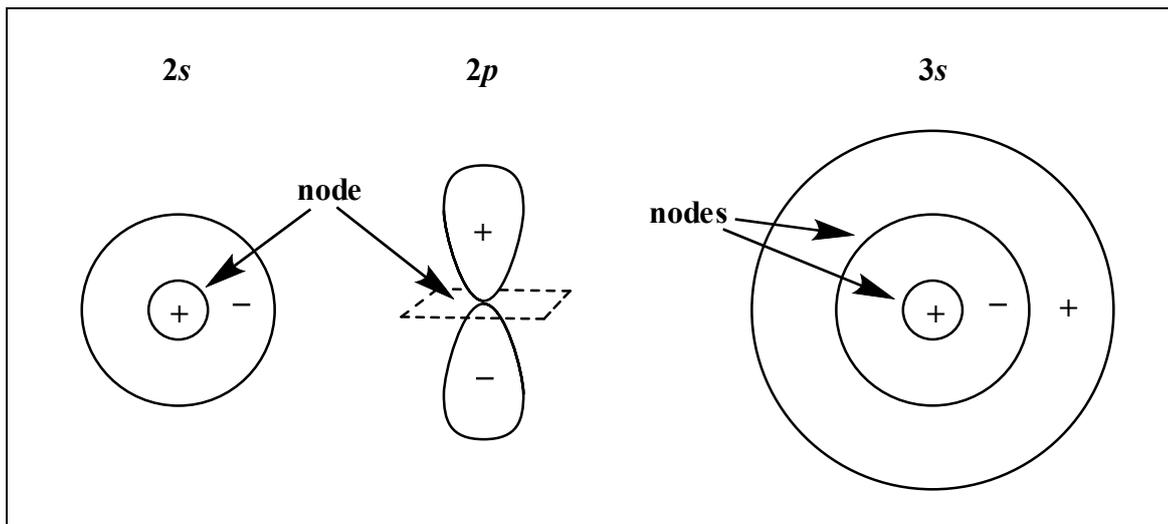
- Explain, with reference to the distribution of electronic energy levels, why crystalline  $\text{SiO}_2$  (quartz) is transparent while crystalline Fe is opaque.

**$\text{SiO}_2$  has no energy states separated by the energy of the photons in visible light, so it does not absorb light in the visible wavelength range and transmits it instead.**

**Crystalline Fe has many energy states separated by the energies of all the photons in visible light, so it absorbs light across the entire visible wavelength range.**

- Describe (or sketch) the shape and arrangement of the nodes in the following three atomic orbitals:  $2s$ ,  $2p$  and  $3s$ .

**Marks**  
2



- Explain the different roles of neutrons and protons in stabilising nuclei.

2

**Long-range Coulomb or electrostatic repulsion between protons acts to push them apart, but the short-range strong nuclear force between all nucleons (protons and neutrons) acts to hold the nucleus together. Neutrons thus contribute to the binding of the nucleus without also contributing to the electrostatic destabilisation.**

- Explain, with reference to the distribution of electronic energy levels, why crystalline  $\text{SiO}_2$  (quartz) is transparent while crystalline Fe is opaque.

2

**$\text{SiO}_2$  has no energy states separated by the energy of the photons in visible light, so it does not absorb light in the visible wavelength range and transmits it instead.**

**Crystalline Fe has many energy states separated by the energies of all the photons in visible light, so it absorbs light across the entire visible wavelength range.**