

Atomic structure

Technology, Information Technology



Tutorial 1: Atomic Structure and Bonding in Solids

1.

- (a) Cite the difference between atomic mass and atomic weight.
- (b) Silicon has three naturally-occurring isotopes as shown in the table below. On the basis of this data, confirm that the average atomic weight of Si is 28.0854 amu.

Silicon Isotope	Natural Abundance	The atomic mass of isotope (AMU)
^{28}Si	92.23 %	27.9769
^{29}Si	4.68 %	28.9765
^{30}Si	3.09 %	29.9738

2.

- (a) Cite two important quantum-mechanical concepts associated with the Bohr model of the atom.
- (b) Cite two important additional refinements that resulted from the wave-mechanical atomic model.

3. Relative to electrons and electron states, what does each of the four quantum numbers specify?

4. Give the electron configurations for the following ions: P^{5+} , P^{3-} , Sn^{4+} , Se^{2-} , I^- and Ni^{2+} .

5. Potassium iodide (KI) exhibits predominantly ionic bonding.

The K^+ and I^- ions have electron structures that are identical to which two inert gases?

6. Without consulting the periodic table, determine whether each of the electron configurations given below is an inert gas, a halogen, an alkali metal, an alkaline earth metal, or a transition metal. Justify your choices.

- a. $1s^2 2s^2 2p^6 3s^2 3p^5$
- b. $1s^2 2s^2 2p^6 3s^2 3p^6 3d^7 4s^2$
- c. $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6$
- d. $1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$
- e. $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6 4d^5 5s^2$
- f. $1s^2 2s^2 2p^6 3s^2$

7. Calculate the force of attraction between a Ca^{2+} and an O^{2-} ion, the centers of which are separated by a distance of 1.5 nm.

8. The net potential energy between two adjacent ions, E_N , may be represented by the sum of the attractive energy, E_A and the repulsive energy, E_R ; Calculate the bonding energy E_0 in terms of the parameters A , B , and n using the following procedure: Differentiate E_N with respect to r , and then set the resulting expression equal to zero, since the curve of E_N versus r is a minimum at E_0 . Solve for r in terms of A , B , and n , which yields r_0 , the equilibrium interionic spacing. Determine the expression for E_N by substitution of r_0 into Equation Q2.

9. For a $\text{Na}^+ - \text{Cl}^-$ ion pair, attractive and repulsive energies E_A and E_R , respectively, depending on the distance between the ions r , according to for these expressions, energies are expressed in electron volts per $\text{Na}^+ - \text{Cl}^-$ pair, and r is the distance in nanometers. The net energy E_N is just the sum of the two expressions above.

- a) Superimpose on a single plot E_N , E_R , and E_A versus r up to 1.0 nm.
- b) On the basis of this plot, determine
- c) the equilibrium spacing r_0 between the Na^+ and Cl^- ions, and
- d) the magnitude of the bonding energy between the two ions.
- e) Mathematically determine the r_0 and E_0 values using the solutions to Question 8 and compare these with the graphical results from part (b).

10.

- (a) Briefly cite the main difference between ionic, covalent, and metallic bonding.
- (b) State the Pauli exclusion principle.

11. Compute the percentage ionic character of the interatomic bond for each of the following compounds: MgO, GaP, CsF, CdS, and FeO.
12. What types of bonding would be expected for each of the following materials: solid xenon, calcium fluoride (CaF_2), bronze, cadmium telluride (CdTe), rubber, and tungsten?
13. Explain why hydrogen fluoride (HF) has a higher boiling temperature than hydrogen chloride (HCl) (19.4°C vs. -85°C), even though HF has a lower molecular weight.
14. Explain why covalently bonded materials are generally less dense than ionically or metallically bonded ones. Asia Pacific University College of Technology and Innovation.