Survey of Materials
Homework 2 – Solution

1. (C,D)

2. There are 4 atoms in the asymmetric unit with coordination number varying from 11 to 16. The interatomic distances vary within the first coordination shell, the five lowest values are 2.24, 2.35, 2.43, 2.52, 2.56 Å. The corresponding APFs are 0.65, 0.75, 0.83, 0.92, 0.98. The distance averaged by no more than 12 nearest neighbors is 2.60 Å, corresponding to APF of 1.02.

3. In hexagonal (trigonal) settings: fcc for $c/a = \sqrt{6}$ ($\alpha = 60°$), sc for $c/a = \sqrt{3/2}$ ($\alpha = 90°$), bcc for $c/a = \sqrt{3/8}$ ($\alpha = 180° - \arccos(1/3) \approx 109°$).

4. (B)

5. (B)

6. Using the compositional identities

$$\frac{AB}{2} = \frac{A}{6} + \frac{A_2B_3}{5}\frac{5}{6}, \quad \frac{A_2B_3}{5} = \frac{AB}{2}\frac{2}{5} + \frac{AB_2}{3}\frac{3}{5}, \quad \frac{AB_2}{3} = \frac{A_2B_3}{5}\frac{5}{6} + \frac{B}{6}$$

we will get the following two-phase mixture energies: $E(AB) = 2.167 < 2.2$, $E(A_2B_3) = 2.26 < 2.4$, $E(AB_2) = 2.333 > 2.3$. Therefore AB_2 decomposes into A_2B_3 and B.

7. (D)

8. (C)

9. Si in SiO_2 can be considered as potential box. The quantized energy levels are $E = \frac{\hbar^2}{2ma^2}\left(n_x^2 + n_y^2 + n_z^2\right)$. The separation between (1,1,1) and (2,1,1) is thus $\Delta E = \frac{3\hbar^2}{2ma^2} \approx \frac{1.1}{m_{\text{eff}}}$ meV. The smallest splitting will be for the highest effective mass which is about 1 in Si.