Point Defects

1. Consider a compound *MX,* where *M* is a monovalent metal cation and *X* is a monovalent, diatomic gas. The material has a bandgap of 5 eV. Also, $g_{Frenkel}$ = 0.5 eV and $g_{Schottky}$ = 3 eV.
    a. Calculate the equilibrium number of both Frenkel and Schottky defects per cubic meter at T = 300K. Which is the dominant internal defect reaction.
    b. Write down the incorporation of X_2 gas in the *MX* material in Kroger-Vink notation.
    c. What are the various Brouwer regimes? Assume the dominant internal defect reaction obtained in part (a) and electronic defects.
    d. At T = 300 K and normal pressure of X_2 gas (say, $p_1 < p_{X2} < p_2$), which Brouwer regime will be active.
    e. Determine the variation of the other defects with p_{X2} in that range of pressure.
    f. Repeat parts d. and e. for $p_{X2} < p_1$
    g. Repeat parts d. and e. for $p_{X2} > p_2$

2. Repeat the above, (a) through (g), for the compound *MX,* where *M* is a divalent metal cation and *X* is a divalent, diatomic gas. The material has a bandgap of 1 eV, and $g_{Frenkel}$ = 2.5 eV and $g_{Schottky}$ = 2 eV.

3. Doping in Si.
    a. Explain the doping of phosphorus and boron in Si using Kroger-Vink notation.
    b. Mg or Ca doping in Si will produce x number of carriers compared to boron doping in Si. What is the value of x? Explain.
    c. Briefly explain why then do we not use Mg or Ca doping in Si.

4. Zn_3P_2 is a material that is gaining lots of attention in recent times as an absorber material for solar photovoltaic conversion as it has the ideal band gap of 1.4 eV. An electronic conductivity experiment at a temperature, T, over a particular range of partial pressure of phosphorus reveals that the slope of ln σ vs ln p_{P4} is 1/8.

a. What is the majority charge carrier in this region?
b. You show this to your advisor and he suggests the following as the compensating defects, singly ionized phosphorus interstitials, singly ionized zinc vacancies, and doubly ionized zinc vacancies. However only one of these is correct, which one?