The Frenkel Defect (also known as the Frenkel pair/disorder) is a defect in the lattice crystal where an atom or ion occupies a normally vacant site other than its own. As a result the atom or ion leaves its own lattice site vacant.

The Frenkel Defect in a Molecule

The Frenkel Defect explains a defect in the molecule where an atom or ion (normally the cation) leaves its own lattice site vacant and instead occupies a normally vacant site. As depicted in the picture below, the cation leaves its own lattice site open and places itself between the area of all the other cations and anions. This defect is only possible if the cations are smaller in size when compared to the anions.

Figure 1: The Frenkel Defect in a molecule

The number of Frenkel Defects can be calculated using the equation:

\[
\sqrt{NN^*} \, e^{\frac{\delta H}{2RT}} \tag{2}
\]

where \(N\) is the number of normally occupied positions, \((N^*)\) is the number of available positions for the moving ion, the delta \(H\) of formation is the enthalpy formation of one Frenkel defect, and \(R\) is the gas constant. Frenkel defects are intrinsic defects because the existence causes the Gibbs energy of a crystal to decrease, which means it’s favorable to occur. [2]

Molecules Found with a Frenkel Defect

The crystal lattices are relatively open and the coordination number is low.

References

Problems

1. What requirements are needed in order for the Frenkel defect to occur in an atom?
2. What are the differences between the Schottky defect and the Frenkel defect?

Answers

1. A low coordination number as well as having the crystal lattices open for the molecule.
2. The Frenkel defect causes an cation to leave its own lattice and go to another, while Sckhotty defect depicts that an equal number of cations and anions must be absent to maintain charge neutrality.

Contributors

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