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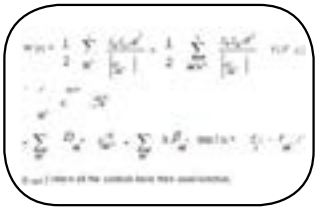
## Modeling and simulation of ground state divalent impurity cat – ion vacancy defect complex

**M Rekha Rani[1], B Srinivasa Rao[2]**
[1]SICET, India
[2]GRIET, India

In the present research work, first time, an attempt has been made to model and simulate the polarization mechanism around a defect complex (Ground State Divalent Impurity Cat-ion Vacancy Defect Complex) using a semi empirical model that goes beyond the phenomenological Born-Mayer type potentials. The present model considers various parameters that constitute and describe the defect lattice and also incorporates many body interactions. Even though the influence of the many body interaction has been studied for simple defects, no attempt has been made for complex defects systems. The present investigation reveals the polarization and its influence on binding energy of the ground state of a Rare Earth divalent impurity and cat ion vacancy defect complex in alkali halide crystal which is a proto-type for ionic solids. For modeling and simulation the three body interaction potential and static simulation technique is used as the static simulation is simple when compared to the ab intio calculations. The computed binding energy reveals that the phenomena of polarization around the defect complex is a responsible factor and governs the stability and ground state configuration of the defect complex. Also, many body interactions are found responsible to enhance the polarization of the complex and in turn to the larger binding energy of the defect complex, in comparison with the general two body potentials. Also the present work stresses the need for better experimental techniques for the study of defect crystal systems in the light of the larger binding energies.

**1. Three Body Potential**

The three body interaction potential can be expressed as

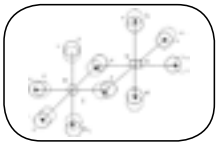


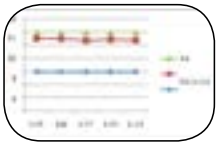
**2.Defect Energy:**

The binding energy (hB) of a divalent impurity cation vacancy complex defect is expressed as $hB = W_0 - W_1$ . Where $W_0$ is the energy required to remove an ion from a real crystal and $W_1$ is the energy necessary to create a vacancy along < 000 > direction in the presence of the divalent impurity at (11).

**3.Samples:** Five divalent impurities of Eu, Mn, Mg, Ca and Ba have considered in NaCl proto-type alkali halides.

**4. Image:** Divalent impurity- Cat-ion Vacancy Defect Complex.





**5. Results:** Formation Energy in ev for divalent impurities in NaCl Proto- Type.

### Biography

M Rekha Rani is pursing PhD in Condensed Matter Physics. *B Srinivasa Rao obtained PhD in Condensed Matter Physics from University of Bhopal, India. He is Professor in Physics and has 60 publications to his credit. His fields of interests are Condensed Matter Physics, Material Science, Neural Networks, Network Security, Cryptology, Wireless Sensor networks etc.

parasar1962@yahoo.in