**Theoretical modeling of point defects in crystals.**

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 Many practical applications of materials are based on the use of the properties caused by point defects, in particular those induced by radiation. Theoretical modeling of defective solids allows one not only explain existing experimental data but also predict the properties of new materials. For low defect concentration it becomes appropriate to model a single point defect in an environment of the remaining solid. In such a  **molecular cluster** model the crystal with a single point defect can be seen as a gigantic molecule and the point defect properties are calculated using any of the methods of the molecular quantum chemistry. There are different possibilities to represent the rest of crystal: embedding into the crystalline environment (**embedded cluster** model), saturation by additional atoms (**saturated-cluster** model). However, in the case of a solid solution the single-defect model is not appropriate as the stoichiometry change is introduced by regular substitution of the host-crystal atoms by those of other chemical species. In this case the point-defect models with periodic boundary conditions (**cyclic cluster** and **supercell**) are more appropriate. These models allow one to use the computer codes and computational methods applied for both the perfect and defective crystals.

 The symmetry aspects and applications of traditional supercell model of defective crystals are considered in [1,2}. Recently a novel **site symmetry approach** for defective crystal calculations in the supercell model was suggested [3]. It is based on the group-theoretical analysis of the site symmetry of the split Wyckoff positions in the perfect crystal supercell, could be applied to a wide class of defects in crystalline solids and allows one to obtain more realistic values for the corresponding point defect formation energy. The efficiency of site symmetry approach was demonstrated for copper impurity in LiCl crystal [2], carbon-doped ZnO crystal [4], oxygen interstitials in corundum [5], polarons in cerium dioxide [6].

References

1. R.A.Evarestov Quantum chemistry of solids. The LCAO first principles treatment of crystals. Springer Series in Solid State Sciences 153, second Edition, Springer, Berlin-Heidelberg (2012)

2. R.A.Evarestov, A.V.Bandura, I.I.Tupitsyn, Theoretical Chemistry Accounts,**137**,14 (2018)

3. R.A. Evarestov , YE Kitaev , VVPorsev , J Appl Crystallogr, **50**,89 (2017)

4. R.A.Evarestov ,S. Piskunov,YF Zhukovskii , Chem. Phys Lett. **682**,91 (2017)

5. R.A.Evarestov, A. Platonenko, D. Gryaznov, YF Zhukovskii,; E.A.Kotomin,; *Phys. Chem. Chem. Phys.* **19**, 25245 (2017)

6.R.A.Evarestov, D.Gryaznov, M.Arrigoni, E.A.Kotomin, A.Chesnokov, J. Maier, Phys. Chem. Chem. Phys. **19**,8340 (2017)