

Localized modes due to H^- in Cesium Bromide

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Abstract— Localized modes due to U-center in Cesium Bromide have been studied by Green function technique. Defect space consisting of impurity atom alone was considered. Using group theory, symmetry coordinates were constructed and analytical expressions were derived for various modes of vibrations in terms of Green's function of the perfect lattice and the perturbation matrix as a result of defect. Mass change at the defect side as well as the change in short range interaction due to the presence of the defect is taken into account. The change in short range force interaction parameter has been compared with changes in this parameter in other Alkali Halides.

Keywords— Localized modes, Green functions, Site symmetry.

I. INTRODUCTION

Vibrational properties of substitutional H^- and D^- impurities have been well discussed in Alkali Halide. Comparatively less studies have been done on the Caesium Halides and this is the motivation for this subject.

II. METHOD OF CALCULATIONS AND RESULTS:

Impurity atom (single atom) defect space was considered.

Considering the symmetry involved, the expression for triply degenerate F_{1U} mode is-

$$\Delta A = [1 - g_0 \epsilon M \omega^2] / 3g_0 \text{-----(1)}$$

$$\text{Here } g_0 = G_{xx}(000, -; 000, -; \omega^2) \text{-----(2)}$$

$$\epsilon M = M_{\text{host}} - M_{\text{defect}} \text{-----(3)}$$

$\Delta A =$ (Parameter A for the defect-host bond) – (Parameter A for perfect lattice)--(4)

$G_{xx}(000, -; 000, -; \omega^2)$ refers to Green function of the perfect crystal

The results are displayed in table 1 along with the experimental values.

Table 1 – Local-mode frequencies of H^- ion in CsBr

ω	A	ΔA
363 (Ref. 2)	8.39 (Ref. 4)	-5.27

ω represents experimental value of local mode frequency in cm^{-1} .

A is the short-range interaction parameter.

ΔA is the change in A, which gives fit to observed frequency.

A and ΔA are in units of $e^2/2V$ of the given crystal (RbBr); e is electronic charge and V is the volume of the unit cell.

III. DISCUSSION

It is seen from the above table that softening in short-range parameter is of the order of 63%. It may be noted that it varies from 8% in KBr : Cl to 64% in KI:Na.

In the present investigation we have just considered impurity atom (1 atom) defect space.

For more realistic computation, one must consider defect space consisting of defect atom and eight nearest neighbours. This work is in progress. It is hoped, our results will find the application in the study of single ion frequency impurities in these crystals.

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