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Interstitial transition atom impurities in silicon: electronic structure and lattice relaxation

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electronic structure and lattice relaxation

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'breathing-mode' relaxation of the surrounding lattice. Electron paramagnetic resonance (EPR) studies suggest (Ludwig and Woodbury 1962, Weber 1983) that most transition atom impurities in silicon occupy the tetrahedral interstitial (TI) site, *preserv-*

Hellmann–Feynman (HF) theorem, the force acting on the pth host ion is then given by

$$\boldsymbol{F}_p(\boldsymbol{Q}) = \int \left(- \nabla_p v_{\mathrm{ps}}(|\boldsymbol{r} - \boldsymbol{R}_p|)\right)\rho(\boldsymbol{r}, \boldsymbol{Q})\mathrm{d}^3\boldsymbol{r} + \sum_{\mu \neq p} \frac{z_p^{\mathrm{H}} z_\mu^{\mathrm{H}}}{|\boldsymbol{R}_p - \boldsymbol{R}_\mu|^3}(\boldsymbol{R}_p - \boldsymbol{R}_\mu) + \frac{z_p^{\mathrm{H}} z^{\mathrm{I}}}{|\boldsymbol{R}_p - \boldsymbol{R}_{\mathrm{I}}|^3}(\boldsymbol{R}_p - \boldsymbol{R}_{\mathrm{I}}), \tag{4}$$

where z_μ^{H} denotes the valence of the host atom at site $\boldsymbol{R}_\mu$ and z^{I} the valence of the interstitial impurity atom. The reason for working in the pseudopotential picture is twofold: (i) it simplifies the calculation of ρ considerably and (ii) the errors in the force

where $K_l^{\alpha\lambda}(\hat{\boldsymbol{r}})$ denotes a Kubic harmonic of order l transforming as the λth partner in the αth irreducible representation of the group T_d. If we define the $l = 1$ projection $\boldsymbol{n}^{(p)}(r)$

in cartesian coordinates,

$$K_0^{a_1}(\hat{\boldsymbol{r}}) = (4\pi)^{-1/2} \qquad K_3^{a_1}(\hat{\boldsymbol{r}}) = (105/4\pi)^{1/2} xyz/r^3$$

$$K_4^{a_1}(\hat{\boldsymbol{r}}) = (21/16\pi)^{1/2}[3(x^2y^2 + x^2z^2 + y^2z^2) - (x^4 + y^4 + z^4)]/r^4 \qquad (20)$$

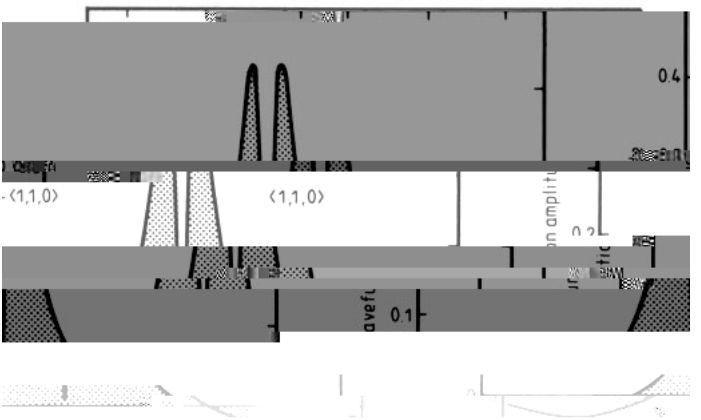

Figure 2. Bound-state wavefunction of e symmetry for Si:Fe in the $\pm\langle 1, 1, 0\rangle$ directions.

indicates the part of the wavefunction which corresponds to around 50% of the normalisation integral. The wavefunction is clearly very atomic-like in the inner CC (almost

4 we show the three lowest radial components of the total charge density $\rho(r)$ (full curves) together with the radial components of the host charge density around the TI site (broken curves). In the direction towards the 1NN at $(a/4)$ (1, 1, 1), where a is the lattice

of atoms around the impurity that are allowed to relax. In these calculations we let the first nine shells around the impurity, corresponding to 82 atoms (or all atoms within a sphere of radius 15 au around the impurity), relax freely while all other atoms are kept in their original positions. We then calculate the equilibrium configuration $\boldsymbol{Q} = \boldsymbol{Q}^*$ of T_d

[redacted]

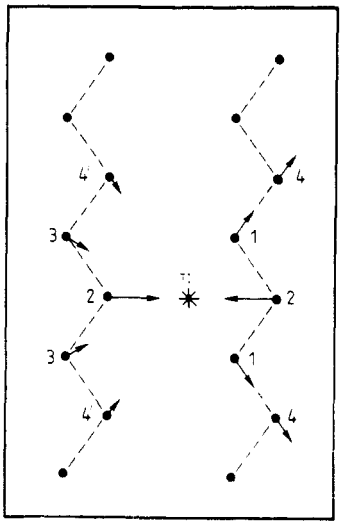

Figure 6. Schematic representation of the displacement of atoms in a $(0, \bar{1}, 1)$ plane. The length of the arrows indicate roughly the relative magnitudes of displacement of the different

value and becomes positive at around $r = 1.5$ au. It turns out that this feature controls the opposite displacements of the 1NN and the 2NN. In figure 9 we have plotted the integrand in equation (13) using the $l = 1$ projected density corresponding to the 1NN. For comparison we have also plotted the integrand using a point-ion potential (broken

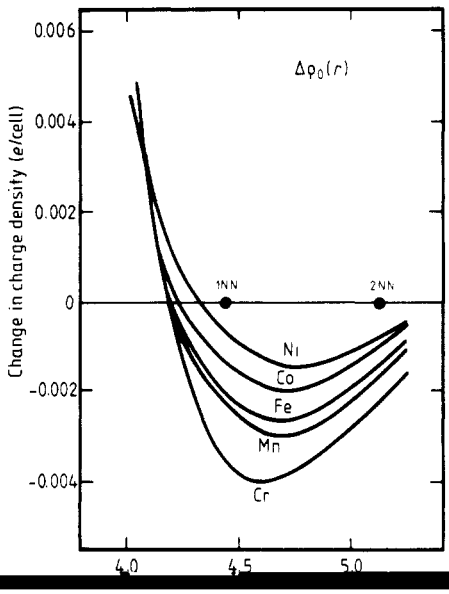

Figure 10. Chemical regularities in the spherically symmetric component of the impurity-induced change in charge density around the first- and

a curve in figure 10 by a parabola, the $l = 1$ projected density magnitude $n_0^{(p)}(r)$ can be calculated analytically. We find that for small r, $n_0^{(p)}(r) = \alpha r$ where $\alpha > 0$ if the atom is situated to the left of the minimum of the parabola and $\alpha < 0$ otherwise. For larger r