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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-*[redacted]

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

$$F_p(Q) = \int (-\nabla_p v_{\mathrm{ps}}(|r - R_p|))\rho(r, Q)\,\mathrm{d}^3 r + \sum_{\mu \neq p} \frac{z_p^{\mathrm{H}} z_\mu^{\mathrm{H}}}{|R_p - R_\mu|^3}(R_p - R_\mu) + \frac{z_p^{\mathrm{H}} z^{\mathrm{I}}}{|R_p - R_{\mathrm{I}}|^3}(R_p - R_{\mathrm{I}}), \tag{4}$$

where z_μ^{H} denotes the valence of the host atom at site R_μ 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 $\boldsymbol{n}^{(p)}(r)$ [redacted]

in cartesian coordinates,

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

[redacted]

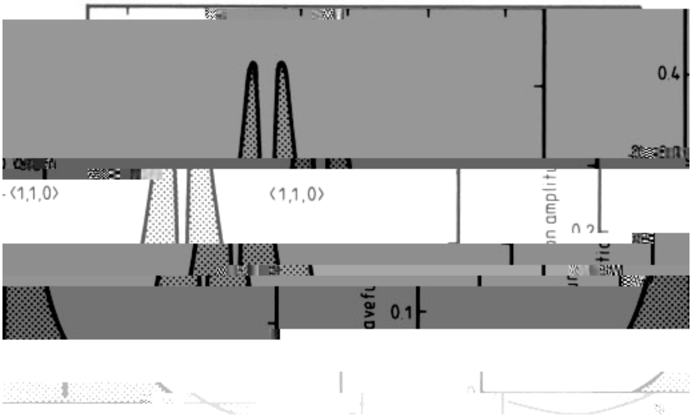

Figure 2. Bound-state wavefunction of e symmetry for Si:Fe in the $\pm\langle 1,1,0\rangle$ directions. The shaded area corresponds to 50% of the normalisation integral.

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

[redacted]

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 $Q = Q^*$ of T_d

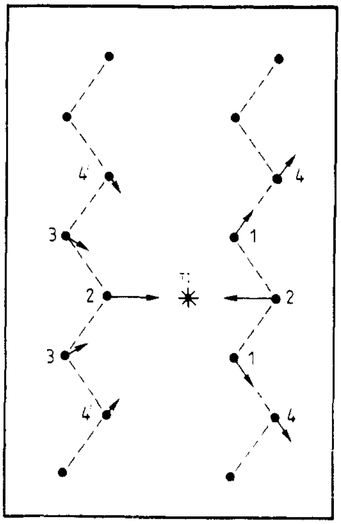

Figure 6. Schematic representation of the displacement of atoms in a $(0, \bar{1}, 1)$ plane. The length of the arrows indicate roughly the relative magnitudes of displacement of the different

[redacted]

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

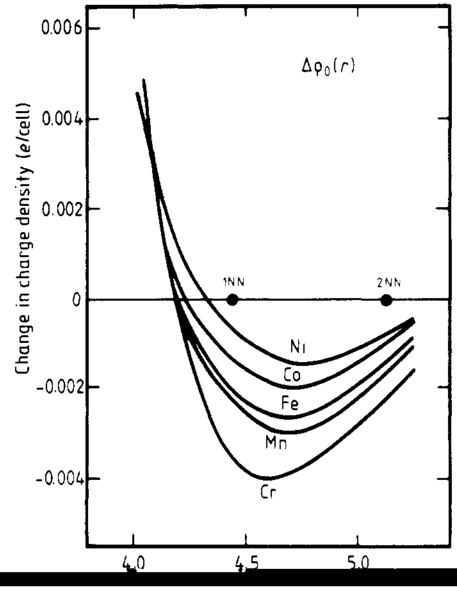

Figure 10. Chemical regularities in the spherically symmetric component of the impurity-induced [redacted]

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

[redacted]