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Breathing-mode relaxation around tetrahedral interstitial 3d impurities in silicon

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The symmetric relaxation of nine shells of host atoms around the tetrahedral interstitial Cr, Mn, Fe, Co, and Ni impurities in silicon are predicted from the self-consistent charge-density displacement and a host-crystal force field. A unique relaxation pattern is predicted

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consistency errors. The first correction measures the amount by which a wave function fails to

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CU

Ct

2.0—

CD

G5

0.0

dv

By 2 PS
cI I'

0.08—

0.06—

0.04—

CC 0.02—

-2.0

0.00—

-0.02-
Q

-0.04

0.0

(D
C3

-0.02—

I I

2NN g= 4

M

(D 0.0 ~

-0.04-

-0.06
Cr Fe Co

FIG. 3. Spherical (I =0) and nonspherical (I =0) contributions to the forces acting on the undistorted first two Si shells around a TM impurity.

I l I I

0.0 1.0 2.0 3.0 4.0 5.0 6.0

Distance (a.u.)
FIG. 2. (a) Host pseudopotential gradients for a paint-core
(———), a soft pseudopotential (Ref. 3) (1), and a hard pseudo-potential (Ref. 11) (2). (b) Magnitude of projected Si-centered den-sity displacement 6 p I ~ (r) for Si:Fe. The insert sho~s the spheri-cally symmetric impurity-centered 5n (r). (c) The integrand of the electronic force [Eq. (2)) acting on the 1NN atom in Si:Fe for a point core (———), and a pseudopotential core {

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). The two
solid circles represent the position of the impurity relative to the 1NN and 2NN Si atom (at the origin).

creasing the attractiveness of AF„leading thereby to an in-ward relaxation. %e conclude that the relaxation pattern of a given host atom is dictated by its relative position in the region where the impurity-induced electronic charge (re-flecting the impurity size) overlaps the non-Coulombic part of the host pseudopotential (reflecting the size of the host atom). The chemical trends for a fixed host are hence dic-tated by the magnitude of the bonding and the antibonding

parts of b, n (r): the heaviest Td (Th488 TdLT)TT /Xi2 outi2 8 Tf 70.53 107.66 Td (0.)Tjj ET11T /Xi2 97.51 Tf 86.11 202.01 Td (dispagnitu44.24 TT11T /Xi2 9 9.81 Tf 168.6 46.61gnitu45d)Tj T11T47 /Xi2 8.59 Tf 180.45 46.5 Td (t47)Tj ET11T47 /Xi27.43 Tf 71.44 155. (conclu49 BT /T11T3T /Xi2bu.8 Tf 99.76 67.03 Tgnituwo)Tj ETT impurity

0.ts

disp8 Td (4

Cg

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