PHYSICAL REVIEVf B VOLUME 27, NUMBER 2 15 JANUARY 1983

Reversal in

REVERSAL IN THE ORDER OF IMPURITY BINDING... 1421

5.0
K
e
~a~
lg

L

0.0
I

CL
0$

~~

e

0
CL
os

E

I

=O("

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4

~

i:
I:
i:
4

~

4

~

i

~

I

~

i

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4

~

4

4.
4:
4'
4.
4

~

4 ~

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4 ~

l:

—2.5

/0

i,
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I,
/o

I:

0.0
$' ~ ~ ra~

- -2.5

eff

ref (r)

C)
s

- 10.0—

6.0

a, gap state

4.0-

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s

2.0-

0.0
-0.2~-"

o / ~

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I ~4

(c)

~ ~' ~
~ ~or ~ ~
'

/ ~Se

- -5.0

imations, as well as early truncations in spectral
sums.

Figure 1(a) displays the r-multiplied pseudopoten-

tial perturbation r 6 Vq"(r) for the s wave of Si:0, Si:S, and Si:Se. As expected from atomic considera-tions, 5

the 0 atom with its deepest atomic s-orbita
energy [IP =28.5 eV (Ref. 9)] has the most attrac-tive b, V", whereas Se with its shallowest atomic s en-

ergy [IP =20.15 eV (Ref. 9)] has the least attrac-tive 6 V" [S is close to Se since its IP is 20.20 eV (Ref. 9)]. The upper panel in Fig. 1(a) shows for these impurities the spherical part (i =0) of the self-consistent screening perturbation. It measures the change in screening potential due to the displace-ment of electronic density in response to 5 V"'. V. Both
rA V

'

and rA V"' attain their asymptotic limits of —2b Z and 2b,Z, respectively, where hZ = 2 is the

difference in valence between the column VI impuri-

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impurity states whose wave functions sample
predominantly region I are likely to have a reversed
order of binding energies relative to impurities with
extended wave functions which are affected predom-
inantly by the potential in region II. As we wi11
shortly see, the orthogonality principle for states of the same angular symmetry (e.g.,

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Since the antibonding state is a donor level and hence derived from the conduction band, it