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compounds was obtained by applying a four-orbital
(s +3p) per atom nearest-neighbor tight-binding

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where the lattice-averaged product of spin variables of

figure fis denoted IIf(o) and reilects the occurrence fre-
quency of this figure in configuration o.

. Df is the degen™

cracy of this figure per fcc site. Table I gives IIf(s) and
Df for the structures' considered by KDF. Assume now that this expansion converges reasonably rapidly and can
be truncated after the inclusion of Xf terms. Specializing
the truncated form of Eq. (7) to a particular set of N, periodic structures [S;I gives

N,

Jf= g [IIf(S,)] 'hH(S,).

f s,.

(9)

To check whether the truncation of the series after Xf
terms is justified, we extract [Jf] through Eq. (9) using
but a small set of only N, =5 (out of 16) structures con-sidered by KDF. These [JfI

values are then used to pre-
dict the energies of the remaining structures [not used in
the inversion of Eq. (9)] from Eq. (8). Comparing the pre-
dicted energies to those calculated directly by tight-
binding provides a measure for the convergence of the
series.

We select a set of N, =5 structures (indicated in Table II by an asterisk) and a corresponding set of Nf =5 in-

f

AH(S;)=Ng IIf(S;)DfJf.
f

Hence, as shown by Connolly and Williams, knowledge of N, =Nf values of b,H(S;) gives N, values of the in-teraction energies,

teractions Jk. These are the normalization term J01, the sites-only term J», and the fcc nearest-neighbor pair J2 „three-body J3 „and four-body J4, interactions.
(Note that the first fcc neighbor equals the second zinc-blende neighbor.) Inverting this 5X5 problem through Eq. (9) gives (in meV)

01 '

~ 11 & 21

(10)
J3 1 0.00625& J41=+0.002 50.

Using these five interactions, we then predict the energies of all remaining structures through Eq. (8). The results are compared in Table II to the values calculated directly by tight binding, showing excellent agreement (after an error in the definition of two structures was identified and

confirmed by B. Koiller). ' Virtually the same results [Eq. (10)] are obtained using any invertible set of five out of 16
structures. We conclude the following.
(i) The tight-binding formation enthalpies calculated by
KDF are internally consistent in that knowledge of about five values suSces to predict the others. The compact

then dictedT /Xi3 10.48 Tf 39126 .33 464.67 4363.33 Td predict of

Comparur 489 ET BT /Xi3 9.15 Tf 340 689 6Tf 422.426.in

of

from

and

Assume

ernally

that enth/Xi3 9.Tf 21448 195meV/ 552.44 Td (and)Tj ET BT /1 Tf 2557883648 195meV/99.67 Td (in)Tj E7T /Xi3 2693 8.8 195meV/(struAssume sn(tin509.33 TdaB /Xi3 /1 Tf 2537.63 195meV/ 552.44509.33 TdaBT /Xi3 /1.01 Tf .4f 4.67 6 Tf 522ymbol94.33 489 Smpact)i3 9.18 2 564.3394.44 Tdfirst u

nf inenth/T /Xi68 411 (8). fd