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These exhibit a rapid decay with nt, in sharp contrast with
the slowly decaying bare Coulomb interactions JJ of Eq.
(2). Comparing Eqs. (2) and (7) we note that whereas
[J;Jj are positive-definite, JF could be either positive or
negative; we find [Eq. (8)] that the dominant effective
first-neighbor term Ji is antiferromagnetic (Ji & 0),
whereas the remaining interactions are ferromagnetic

(J & i & 0). The fcc Coulomb lattice is hence frustrated. The rapid convergence and practical completeness of this set [JF] allows us to calculate the configuration aver-

age (Est)tt =—Est(R) for the random alloy. Using in Eq.
(4) the configurationally averaged pair correlation func-
tions &IIF&tt (2x —1) appropriate to the random alloy,
we find ast(R, x) 0.73865 [4x(1—x)], in excellent agreement with the analytic result ast(R, x) 0.73952 [4x(1—x)], which can be obtained by substituting Eq.
(3) into Eq. (I) and evaluating explicitly its con-figurational average. The excellent agreement between the analytic result and that of the truncated cluster expan-sion lends credence to the latter

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EM(rr)

=- &zag
d

aM (o')ag '
2p'

PM (rJ)~gg
d

(lo)
where aza 1.638055 is the Madelung constant of the zinc-blende (ZB) lattice, PM(o') 4aza[x(a) —0.5), d v3/4a is the nearest-neighbor anion-cation distance, and asr(o) is a geometrical constant to be calculated
below.

We have repeated for A~-„B„C(Table II) the same
procedure used above for A~ „8„. The results are given

in Table II. We see that the predicted values for ordered structures agree very well with those calculated directly by Ewald's method, and that the result aM(R, x 0.5) 2.51643 for the random pseudobinary alloy also agrees well with the exact value asr (R,x 0.5) 2.51599.

Unlike the case in binary A~ „8,alloys, the dominant

The charges on the different C atoms are then decided by the electroneutrality condition for each C-centered

A„84 „(0~n~4) tetrahedron. This gives the charge
distribution for 8 & —„B„Calloy as
Q; =Q+Ag S; (i in the A,B sublattice)
(9)

Qj = —Q+ gS; (j in the C sublattice),

l

where Q (Qg+Qa)/2, hg (Qa —gg)/2, and S J

is

the spin variable for the occupation of the four tetrahedral

vertices i centered at j. Using Eq. (9), the Madelung en-ergy of the A ~ „B„Cs—emiconductor lattices can be ex-
pressed as

effective interactions in pseudobinary A&-„B„Csystems (given in the caption to Table II) are found to be fer-romagnetic, hence, the ground state corresponds to phase
separation. This reflects the fact that the (negative)
Madelung energy of A ~ „B„Cis minimal for the AC and
BC constituents, since, relative to the average charge
value (LLQ -0) the constituents exhibit the largest charge
fluctuation (+ d,g) on the common sublattice C. Note
that the trend of stability of (AC)„(BC)„superlattices predicted by this model (i.e., [111]structures have the
next lowest energy after the phase-separated system) is
consistent with first-principles total-energy calculations for lattice matched semiconductor superlattices. '
In summary, we have shown that cluster expansion used previously in numerous calculations of phase diagrams'7
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