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Invited

Predictions of New Semiconductor of Transition Metal Structures and Their Properties

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I describe how one can use the "Cluster Expansion Method" to predict systematically what are the thermodynamically stable crystal structures on a given lattice type. The method is used to illustrate how hitherto unsuspected ordered com-

pounds can be identified, including [illegible]

I will discuss here the prospects of the recently developed "cluster expansion methods"[6] which allow one to (i) perform a systematic ground state search among 10^5

atomic configurations and, (ii) obtain the temperature-composition phase diagram in a *first-principles manner*,

system.[13] For example, information about the values of the J's may be extracted from experimental critical temperatures.[13] This approach is the simplest, but it provides

little new information about the properties of the alloy. *The second approach* is to determine the J's by treating same composition, as well as the stability of the

50% equimolar compounds exhibit at low temperatures a metries established clearly from experiment[24] are also

ted from the basis set used to extract J_F some of the struc-

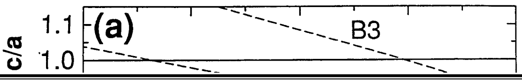
layer $(AC)_1/(BC)_1$ superlattices in the (111) orientation[32]

never perfect; it can however, be maximized in certain predicted to alter the alloy's band structure [illegible]

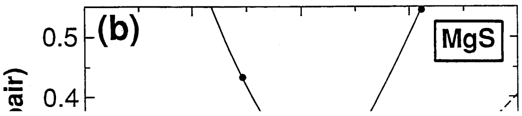
reduction depends (quadratically) on the degree η of long grown on GaAs[42] (rather than the alloy). There are now experimental confirmations of this idea.[43] (ii) Use of strain to convert the *indirect* gap Si_nGe_n SL grown on Si

The terms in brackets are the nearest-neighbor terms of eq. (3). All odd terms were omitted, assuming that the Hamiltonian is invariant under the A↔B interchange.

[Fig. 6(b)]. The maximum equilibrium solubility of ZnSe in CuInSe$_2$ with the chalcopyrite structure is 22% (at T = 770 K) while CuInSe [illegible]



order temperature of CuInSe$_2$. Our results hence show that, contrary to the other known heterostructural ternary alloy (GaAs)$_{1-x}$Ge$_{2x}$, characterized by vanishing solid solubility (CuInSe$_2$)$_{1-x}$(ZnSe)$_{2x}$ should exhibit substan- [illegible]



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24) P. M. Hansen: *Constitution of Binary Alloys* (McGraw-Hill, New York, 1958).