terms). If the series Eq 3 converges after M terms, one can calculate an equivalent number of interaction energies $\{J_f(V)\}$ by equating Eq 2 with Eq 3. For example, the simplest, direct in-

M

σ

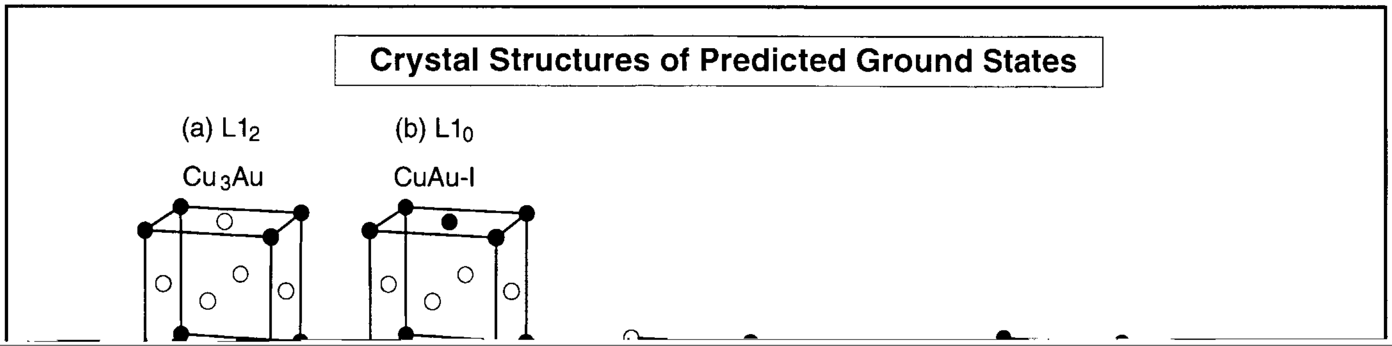
which can be obtained once one has performed self-consistent quantum-mechanical calculations on M different A_nB_m ordered structures. These structures do not have to be ground

nuity in the internal energy as a function of temperature and the ground state determined by the state of the simulation at a temperature where all configurational changes proved to be ener-

The Warren-Cowley SRO parameter[46] for the Nth atomic shell at distance R_l from the origin is:

$$\alpha_{\mathrm{SRO}}(R_{lmn}) = \frac{<\Pi_{0,N}> - q^2}{1 - q^2} \qquad \text{(Eq 7)}$$

where $q = 2x - 1$, and the angular bracket denotes a configura-



Crystal Structures of Predicted Ground States

4. Conclusion

Using a first-principles quantum-mechanical method (which properly includes the terms that were neglected by the previous theories, such as simplified tight-binding Hamiltonian

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