Mixed-Basis Cluster Expansion for First Principles Alloy Thermodynamics

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The Mixed-Basis Cluster expansion represents the total energy of substitutional lattice configuration via a reciprocal-space description of all pair interactions and a real-space description of the many-atom terms.The K 0 singularity due to atomic mismatch strain is correctly included via the Coherency-strain term .The parameters of this expansion– the pair,many-atom,and strain terms are obtained from LDA calculations on a few ordered compounds. This approach permits a flexible description of metal alloys,semiconductor alloys and insulator alloys with any atomic size mismatch or charge-transfer. I will show how the choice of structures and interactions can be decided from optimization algorithms. Once the expansion is fit to LDA ,it is effectively coupled to Monte-Carlo simulated-annealing algorithm.This gives (a) Ground state structures (b) Short- range-order (c) Finit temperature thermodynamic functions and (d) alloy micro structures,e.g precipitate shapes,orderind domains.

I will illustrate the method for a few recently calculated cases (as time permits), including Al-Zn precipitates,Cu-Au ordering domains,Phase stability of Ag-Pd,Cu-Pd,Cu-Au,Ni-Au,Cu-Zn ,and vacancy ordering in transition metal sulphides.