

Special Quasirandom Structures

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Substitutional alloys are disorder crystalline structure. First-principles study of alloys is take a large supercell that equivalent to a pure random structure. Structural models used in calculations of properties of substitutional random $A_{1-x}B_x$ alloys are usually constructed by randomly occupying each of the N sites of a large periodic supercell by A or B . However this method is not efficient. But there is a way that it is possible to design "Special Quasirandom Structures"(SQS) that simulate the small periodic supercell. It can be compared to structures that have large number of configurations or large cell sizes. The proposed method optimizes the supercell with the occupation of the atomic sites (A or B). Using the language of Ising models to define the product of spin variable for each atomic sites. Then calculate a lattice average to construct special periodic quasirandom structures that can be used in the calculating total energy, optical and thermodynamic properties.

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