

Nowotny Chimney Ladders and Giant Cubic Structures: Electron Driven Interfaces

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Sometimes intermetallic phases can adopt bewildering structures with hundreds or thousands of atoms per unit cell, or no detectable 3-dimensional periodicity. Using quantum mechanical calculations as a guide to view these structures, we will see one reason that such structures form: many complex intermetallics are, at heart, simple structures that have made room for extra electrons through the formation of interfaces. The Nowotny chimney ladder phases are an example: these are beautiful examples of two component composite crystals, in which the two incommensurable components form helical motifs. Electronic structure calculations reveal that the complex chimney ladder structures each chimney ladder consists of slabs of TiSi_2 structure type. The interfaces between the slabs act as electron sinks to achieve electron counts optimal to the TiSi_2 structure. The same thing happens in giant cubic intermetallic phases based on Friauf polyhedra, such as NaCd_2 . This phase the NaCd_2 structure, with over 1000 atoms per unit cell, is also built from blocks cut from a simple structure type, this time the MgCu_2 type. Extra electrons are accommodated by the interfaces between MgCu_2 -type blocks. While in the chimney ladders, the blocks are separated by planar interfaces, the interfaces in NaCd_2 form a minimal surface, the P surface.

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