

Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Small to medium atomic size mismatch leads to phase-separation yet very large mismatch can lead to spontaneous ordering.¹ MAYEUL D'AVEZAC, XIUWEN ZHANG, NREL, GIANCARLO TRIMARCHI, Northwestern University, ALEX ZUNGER, NREL — Large atomic size-mismatch between compounds discourages their binding onto a common lattice because of the ensuing cost in strain energy. This central paradigm in the theory of isovalent alloys, is clearly broken by the occurrence of stable spontaneous long-range order in mixtures of alkali-halides with as much as 40% size-mismatch (e.g LiF-CsF). Our theoretical analysis of these failures uncovered a different design principle for stable alloys: very large atomic size-mismatch can lead to spontaneous ordering if the large (small) components have the ability to raise (lower) their coordination number (CN) within the mixed phase. This heuristic design-principle leads us to explore via first-principles structure-search a few mismatched binary systems whose components have a propensity for CN disproportionation. We find ordered structures for BeO-BaO (37% size-mismatch) and BeO-SrO (30%), and ordering in LiCl-KCl (20%). BN-InN (33%) lowers its positive formation enthalpy by 60% with CN disproportionation. This design principle could be used to explore novel phases not expected to order according to the common paradigm of strain instability.

¹Funded in part by Energy Frontier Research Center for Inverse Design.

Mayeul d'Avezac
NREL

Date submitted: 20 Nov 2009

Electronic form version 1.4