Abstract Submitted
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Small to medium atomic size-mismatch leads to alloy phase-separation yet huge mismatch can lead to ordering[1] XIUWEN ZHANG, GIANCARLO TRIMARCHI, MAYEUL D'AVEZAC, ALEX ZUNGER, National Renewable Energy Lab., Golden, CO 80401 — Most alkali halide alloys AX-BX (where A and B are alkali elements and X=F, Cl, Br, or I) are expected to have miscibility gaps (phase separation) which increases with the lattice mismatch. Even though LiX-RbX and LiX-CsX with lattice mismatches of $20-33\%$ and $19-40\%$ respectively might be expected to have pronounced miscibility gaps, they were experimentally found to have ordered structures. Here, we investigate the possible stabilization of ordered compounds with respect to random configurations. In the family of $LiNaBr_2$, $LiKBr_2$, $LiRbBr_2$, and $LiCsBr_2$, we find that as the lattice mismatch increases, the formation enthalpy of the random structure increases, (mainly due to the volume deformation), but the formation enthalpy of the ordered structure decreases becoming negative for the latter two. The ordered structures consist of distorted LiX4 tetrahedral arranged in layers, with Rb (or Cs) sitting between layers at the center of the resulting triangular prism. We analyze the origin of ordering from the large local distortion induced by the huge lattice mismatch.

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