Charge Transfer Electrostatic Model of Compositional Order in Perovskite Alloys*

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We use an electrostatic model including charge transfer to study compositional ordering in perovskite alloys with A-site and B-site doping. The method [1] generalizes the approach of Bellaiche and Vanderbilt [2], who used nominal ionic charges. The large covalency of Pb^{2+} compared to Ba^{2+} is modeled by an environment dependent effective A-site charge. Monte Carlo simulations of this model reproduce the long range compositional order of both Pb-based and Ba-based $A(BB^{'}B^{''})O_3$ perovskite alloys as a function of temperature and B^{4+} concentration. In systems with both A- and B-site doping, such as $(Na_{1/2}La_{1/2})(Mg_{1/3}Ta_{2/3})O_3$, $(Ba_{1-x}La_x)(Mg_{(1+x)/3}Nb_{(2-x)/3})O_3$ and $(Pb_{1-x}La_x)(Mg_{(1+x)/3}Ta_{(2-x)/3})O_3$ [3], purely electrostatic interactions reproduce general trends, and charge transfer effects indicate that local structural relaxations can tip the balance between different B-site orderings in Pb based materials.

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