

Abstract Submitted  
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**Configurational Electronic Entropy and the Phase Diagram of Mixed-Valence Oxides: The Case of  $\text{Li}_x\text{FePO}_4$**  FEI ZHOU, THOMAS MAXISCH, GERBRAND CEDER, Department of Materials Science and Engineering, MIT — We demonstrate that configurational electronic entropy, previously neglected, in *ab initio* thermodynamics of materials can qualitatively modify the finite-temperature phase stability of mixed-valence oxides. While transformations from low-T ordered or immiscible states are almost always driven by configurational disorder (i.e. random occupation of lattice sites by multiple species), in  $\text{FePO}_4$ – $\text{LiFePO}_4$  the formation of a solid solution is almost entirely driven by electronic, rather than ionic configurational entropy. We argue that such an electronic entropic mechanism, rather than an ionic one, may be relevant to most other mixed-valence systems. Details in Phys. Rev. Lett. **97**, 155704 (2006)

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