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Temperature - Concentration Phase Diagram from First Principles Calculations in P2-Na_xCoO_2[1] YING S. MENG, University of Florida, YOYO HINUMA, GERBRAND CEDER, Massachusetts Institute of Technology — The unusual electronic and magnetic properties of Na_xCoO_2 are attracting considerable interest in recent years. At high sodium content, the system displays unusually strong thermoelectric effect and a low metallic resistance. In this paper, we present temperature - concentration phase diagram for Na_xCoO_2 (0.5 <= x <= 1) obtained with first principles method of the Density Functional Theory (DFT) in the Generalized Gradient Approximation (GGA) scheme, where charge on Co is delocalized. In comparison we will also present the results obtained from the GGA with Hubbard U correction (GGA+U) scheme, where charge on Co is completely localized, forming Co^{3+} and Co^{4+}. The stable Na-vacancy ordering schemes at various concentrations obtained in this work will be compared and contrasted with available experimental observations. We will discuss the key interactions that determine the ground states and the order/disorder transition temperatures of these states, which is important for understanding the thermoelectric properties of these mixed valence oxides.

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