

# DEFECT ANALYSIS AND THERMODYNAMIC MODELING OF $\text{LaCoO}_{3-\Delta}$

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**Abstract:** The defect structures of the  $\text{LaCoO}_{3-\delta}$  perovskite are analyzed through thermodynamic modeling by means of the CALPHAD technique. Based on available experimental data, a compound-energy model, i.e.  $(\text{La}^{3+}, \text{Va})_1(\text{Co}^{2+}, \text{Co}^{3+}, \text{Co}^{4+}, \text{Va})_1(\text{O}^{2-}, \text{Va})_3$ , is proposed. It is discovered that charge disproportionation exists for  $\text{Co}^{3+}$  in order to describe the relationship between the oxygen partial pressure and the oxygen deficiency. It was consequently predicted that the amounts of  $\text{Co}^{2+}$  and  $\text{Co}^{4+}$  are about 20% each when there is no oxygen deficiency.