"Synthesis, Optical, Magnetic and Thermodynamic Properties of Rocksalt $Li_{1.3}Nb_{0.3}Mn_{0.4}O_2$ Cathode Material for Li-Ion Batteries"

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Abstract

Since the discovery of the reversible intercalation of lithium-ion materials associated with promising electrochemical properties, lithium-containing materials have attracted attention in the research and development of effective cathode materials for lithium-ion batteries. Despite various studies on synthesis, and electrochemical properties of lithium-based materials, fairly little fundamental optical and thermodynamic studies are available in the literature. Here, we report on the structure, optical, magnetic, and thermodynamic properties of Li-excess disordered rocksalt, Li1.3Nb0.3Mn0.4O2 (LNMO) which was comprehensively studied using powder X-ray diffraction, transient absorption spectroscopy, magnetic susceptibility, and low-temperature heat capacity measurements. Charge carrier dynamics and electron–phonon coupling in LNMO were studied using ultra-fast laser spectroscopy. Magnetic susceptibility and specific heat data are consistent with the onset of long-range antiferromagnetic order at the Néel temperatures of 6.5 (1.5) K. The effective magnetic moment of LNMO is found to be 3.60 mB. The temperature dependence of the inverse magnetic susceptibility follows the Curie–Weiss law in the high-temperature region and shows negative values of the Weiss temperature 52 K (3), confirming the strong AFM interactions.

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