Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Structure prediction and phase diagram calculation of NaxCoO2 by Ab Initio methods YING SHIRLEY MENG, YOYO HINUMA, OSMAN BURAK, GERBRAND CEDER, Massachusetts Institute of Technology, DEPARTMENT OF MATERIALS SCIENCE AND ENGINEERING, M.I.T. TEAM — The unusual electronic properties of NaxCoO2 make it a material of considerable interest. At high sodium concentration it displays a remarkable combination of high electronic conductivity and high Seebeck coefficient. Understanding these phenomena requires a detailed understanding of the local structure, since different Na-vacancy orderings are strongly coupled to the electronic structure and Co3+/Co4+ arrangement. In this study, we investigate the charge ordering and Na-vacancy ordering using first principles electronic structure methods within the GGA and GGA+U approximations. Na ordering is determined not only by a competition between Na site energies difference and Na-Na repulsion, but also by the Co-Na interlayer interaction induced by charge localization. We believe that in particular at high Na content a quantitative understanding of the coupling is essential in understanding the remarkable electronic properties. Phase diagram calculations of NaxCoO2 to understand the phase stability in the system will be presented.

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Date submitted: 08 Nov 2006 Electronic form version 1.4