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Theory of Sodium Ordering in Na_xCoO_2 STEVEN G. LOUIE, PEI-HONG ZHANG, MARVIN L. COHEN, U. C. Berkeley and LBNL, RODRIGO B. CAPAZ, Universidade Federal do Rio de Janeiro, U. C. Berkeley and LBNL — The ordering of Na ions in Na_xCoO_2 is investigated systematically over the full range of doping by combining detailed density functional theory (DFT) studies with model calculations. Various ground state ordering patterns are identified and are in excellent agreement with available experimental results. Our results suggest that the primary driving force for the Na ordering is the screened electrostatic interaction among Na ions. Possible effects of the Na ordering on the electronic structure of the CoO_2 layer are discussed. We propose that the nonexistence of a charge ordered insulating state at $x = 2/3$ is due to the lack of a commensurate Na ordering pattern, whereas an extremely stable Na ordering at $x = 0.5$ enhances the charge ordering tendency, which results in an insulating state as observed experimentally. RBC acknowledges financial support from the John Simon Guggenheim Memorial Foundation and Brazilian funding agencies CNPq, CAPES FAPERJ, Instituto de Nanociências, FUJB-UFRJ and PRONEX-MCT. Work partially supported by NSF Grant No. DMR00-87088 and DOE Contract No. DE-AC03-76SF00098. Computational resources were provided by NPACI and NERSC.

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