

Abstract Submitted
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Modelling sodium cobaltate by mapping onto magnetic Ising model¹ PATRICK GEMPERLINE, DAVID JONATHAN PRYCE MORRIS, Xavier University, Cincinnati, OH — Fast Ion conductors are a class of crystals that are frequently used as battery materials, especially in smart phones, laptops, and other portable devices. Sodium Cobalt Oxide, Na_xCoO_2 , falls into this class of crystals, but is unique because it possesses the ability to act as a thermoelectric material and a superconductor at different concentrations of Na^+ . The crystal lattice is mapped onto an Ising Magnetic Spin model and a Monte-Carlo Simulation is used to find the most energetically favorable configuration of spins. This spin configuration is mapped back to the crystal lattice resulting in the most stable crystal structure of Sodium Cobalt Oxide at various concentrations. Knowing the atomic structures of the crystals will aid in the research of the materials capabilities and the possible uses of the material commercially.

¹Ohio Supercomputer Center. 1987. Ohio Supercomputer Center. Columbus OH: Ohio Supercomputer Center. and the John Hauck Foundation

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