Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

First Principles Study of Misfit-Layered Calcium Cobaltite Using Fibonacci Approximants[1] ALEJANDRO REBOLA, ROBERT KLIE, SERDAR OGUT, University of Illinois at Chicago — Cobalt oxides have been the focus of many recent studies due to the wide variety of electrical, magnetic, structural and thermoelectrical properties they exhibit. In this talk we present a first-principles study on the misfit-layered $Ca_3Co_4O_9$. This material can be more accurately described as $[Ca_2CoO_3][CoO_2]_{1.61}$ and consists of two substructures that are incommensurate to each other. Taking into account that the composition ratio is very close to the golden mean (1.6180...), and that this number can be obtained as the limit of the sequence of the ratios of consecutive Fibonacci numbers: 3/2, 5/3, 13/8, ..., F(n+1)/F(n)..., we model the structure by using supercells of composition $[Ca_2CoO_3]_{F(n)}[CoO_2]_{F(n+1)}$. In this way, structural, electronic, transport and lattice properties can be calculated as a function of cell size. We compute the atomic and electronic structures, defect energetics of a series of rational approximants to $Ca_3Co_4O_9$within the framework of DFT+U, and examine the convergence of such properties with respect to size, thus allowing us to identify the most realistic and smallest structural model for this misfit-layered compound.

[1]This work is in part supported by the US Army Research Office (W911NF-10-1-0147).

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Date submitted: 22 Dec 2010 Electronic form version 1.4