Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Crystal structure and electronic properties of the oxygen deficient $Sr_3Ru_2O_{7-y}$ ($0 \leq y \leq 0.5$) ruthenate OLIVER MARTINEZ-ANAYA, GUSTAVO TAVIZON, Facultad de Quimica, PABLO DE LA MORA, Facultad de Ciencias, ROBERTO ESCUDERO, Instituto de Investigacion en Materiales, Universidad Nacional Autonoma de Mexico — In this work a study of the structural properties of the new non-stoichiometric Ruddlesden-Popper type $Sr_3Ru_2O_{7-y}$ compounds is presented. $Sr_3Ru_2O_{7-y}$ (y = 0.17, 0.23, 0.28, 0.40 and 0.47) were synthesized by hydrogen reduction of the parent $Sr_3Ru_2O_7$ ruthenate. Rietveld structure refinements were performed to determine the crystal structure of the reduced compounds. Oxygen content of the samples was studied by redox chemical titration and ESR spectra confirmed the presence of Ru^{3+}. Removal of oxygen atoms from the parent compound results in shrinkage of the c and growing of the a lattice parameters, which we related to the Ru^{4+} to Ru^{3+} partial reduction in $Sr_3Ru_2O_7$. On basis of DFT calculations, with WIEN2k code, we compared the electronic properties of reduced and stoichiometric compounds.

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Date submitted: 23 Dec 2011 Electronic form version 1.4