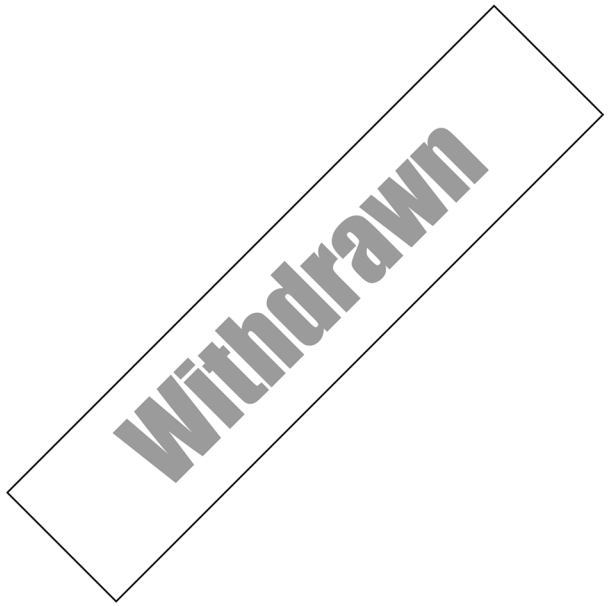
AC02



AC03

Electronic Structures and Magnetic Properties of Spin-Lattice Coupled Systems

B. I. Min*

Department of Physics, Pohang University of Science and Technology, Pohang 790-784, Korea

*Corresponding author: e-mail: bimin@postech.ac.kr

Perovskites and spinels of recent interest, which are candidates for the next generation spintronic materials, manifest the complex interplay of the spin and other lattice degrees of freedom. The lattice here is meant by the degrees of freedom other than the spin such as the charge, orbital, as well as real lattice vibration. The dominant magnetic interaction in those spin-lattice coupled systems is the superexchange interaction between transition metal ions through intervening anion (e.g. oxygen, sulphur ions). The superexchange interaction depends strongly on details of the material properties such as the electron occupancy, orbital configuration, and the geometric arrangement. The systematic study on the microscopic mechanism is lacking, and the discussion often relies on the phenomenology like Goodenough-Kanamori-Anderson (GKA) rule in many cases. In this study, based on the results from the first principles band methods, we investigate the effects of the spin-lattice coupling on the electronic, magnetic, structural properties of several materials including perovskite $SeCuO_3$, La_2NiMnO_6, spinel $FeCr_2S_4$, MnV_2O_4, and Po. We discuss the electronic and magnetic properties of the above perovskite and spinel compounds, and explore the origin of the stabilized simple cubic structure for Po.