Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Electronic and Magnetic Properties of Ba, Ni and $BaNiO_3$: A First-Principles Study RUPESH GHIMIRE, GoldenGate International College, NARAYAN ADHIKARI, GOPI KAPHLE, Tribhuvan University, RAMESH MANI, Georgia State University — The electronic and magnetic Properties of Ba, Ni and hexagonal crystal structure $BaNiO_3$ have been studied under TB-LMTO ASA method. The space group of compound is $P6_3/mmc$ and lattice parameters are a=b=5.62 A° and c=4.81 A°. From our calculation, the minimized lattice parameters of Ba, Ni and $BaNiO_3$ were found to be 5.280 A°, 3.488 A° and 6.08 A° which are at most 1% deviation from the experimental values. Band Structures were determined using the minimized structures which showed the metallic nature of elements Ba and Ni. However, the compound $BaNiO_3$ possessed a band gap of 0.95 eV under LDA calculation. Further, U correction was implemented to account for the orbital dependent potential arising largely from the strong correlation of d and f electrons, and the band gap increased to 1.59 eV which is close to the theoretically expected gap (1.612 eV). Density of states showed the ferromagnetic nature of the element nickel with a magnetic moment of $0.59\mu_B$ close to that of experimental $0.60\mu_B$, whereas the compound $BaNiO_3$ itself was non-magnetic. Finally, a brief study of the charge properties showed the presence of ionic and covalent bonds between the atoms.

Ramesh Mani
Georgia State University

Date submitted: 10 Nov 2016 Electronic form version 1.4