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A First Principle exploration of A site ordered $Ho_{0.5}A_{0.5}MnO_3$(A=Ge, Sn, Pb, As, Sb, Bi, Se, Te) SATHYA SHEELA SUBRAMANIAN, National Institute of Technology, Trichy, India, Japan Advanced Institute of Science and Technology, Japan, TAISUKE OZAKI, Japan Advanced Institute of Science and Technology, Japan, KUNIHIKO YAMAUCHI, ISIR-SANKEN, Osaka University, Japan, NATESAN BASKARAN, National Institute of Technology, Trichy, India, TAMIO OGUCHI, ISIR-SANKEN, Osaka University, Japan — In this work a first principle attempt has been made to study the structure and properties of doping lone pair cations to ortho-$HoMnO_3$. Electronic structure calculations were carried out to study $Ho_{0.5}A_{0.5}MnO_3$ (A=Ge, Sn, Pb, As, Sb, Bi, Se, Te) under the Generalized Gradient Approximation of Density Functional Theory in an attempt to analyze the effect of lone pair cations towards electric polarization and to predict new multiferroics. Under the first principle calculations, $Ho_{0.5}A_{0.5}MnO_3$ (A=Ge, Sn, As, Sb, Bi, Se, Te) is found to be multiferroic. Doping 50% of Se and Sn to $HoMnO_3$ is found to highly enhance the electric polarization compared to parent ortho-$HoMnO_3$. O2p- A valence p orbital hybridization is expected to be the cause of this polarization. Thus $Ho_{0.5}Se_{0.5}MnO_3$ and $Ho_{0.5}Sn_{0.5}MnO_3$ are expected to be good candidate multiferroics. A first principle attempt has thus been made to perform an extensive search for new multiferroics in which p-p hybridization is found to have a strong role in causing electric polarization predicting new multiferroics providing a pathway for experimentalists to synthesis new promising multiferroic compounds.

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