Abstract Submitted
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Study of p-type behavior in NiO doped Cu and Ag using ab initio calculations[1] SAMUEL CANTRELL, LUISA SCOLFARO, Texas State University, PABLO BORGES, Universidade Federal de Vicosa, WILHELMUS J. GEERTS, Texas State University — NiO has become an active area of research due to it's potential to be used in the next generation of Resistive RAM (RRAM) devices. Thus it is of interest to study how this material behaves in response to introduced impurities in order to ascertain if the doped system improves desired properties. To that end, we have used Density Functional Theory (DFT) together with the VASP-PAW method based ab initio calculations to study the effects of introducing Cu and Ag atoms via replacing Ni into pristine NiO. Exchange-correlation effects were included in the calculations within the generalized gradient approximation (GGA). To better describe the d-orbitals of Ni, Cu, and Ag, a Hubbard potential U contribution was added (GGA+U), in all systems studied. Preliminary results also considering a hybrid functional (HSE06) to treat the exchange correlation are shown. The pristine and doped NiO systems were studied using supercells grown along the [111] direction of 4 and 32 atoms in order to simulate antiferromagnetic configurations for the pure NiO and doped systems respectively. Concentrations of Cu and Ag of 6.25

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