Abstract Submitted
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First principles study of oxygen vacancies and iron impurities on electrical and optical properties of NiO[1] JOHN PETERSEN, TWAGIRAYEZU FIDELE, Texas State University, PABLO BORGES, Universidade Federal de Viosa, Brazil, LUISA SCOLFARO, WILHELMUS GEERTS, Texas State University — We are studying the properties of iron doped NiO by Density Functional Theory. NiO is being considered for use in RRAM, based on the reversible switching of a thin transition metal oxide (TMO) layer between a low and high resistance state using the mechanism of soft breakdown. RRAM's high integration density, its high endurance and good retention, its low energy use, and its high speed make it a potential candidate for replacing Flash memory. Switching between the high and low resistance state is inhomogeneous, and low resistance nano-filaments are formed. Fe impurities are introduced to optimize the switching properties. The effects of oxygen vacancies and iron on the electronic structure and optical properties of NiO are calculated and compared with experiment. Antiferromagnetic rhombohedral 108 atom cells with 1.85% Fe concentration are considered. Due to the highly-correlated nature of d orbitals in TMOs, a Hubbard U correction is applied to calculations in this work via the GGA + U method of DFT using VASP. Hybrid HSE06 calculations will also be considered. Localized energy levels from iron and from oxygen vacancies are identified, and their effects on dielectric permittivity are presented.

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