**Ab initio Study of Structural and Electronic Properties of Rare-Earth Nickelates**

K.Z. Rushchanskii, S. Blügel, and M. Ležaić  
Peter Grünberg Institut, Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425, Jülich, Germany

**MOTIVATION**

Ability of switching between metallic and insulating states by external factors is a very demanding property for industrial applications such as ferroelectric memories. In this sense, rare-earth nickelates are very promising materials due to their perovskite crystalline structure, which allows epitaxial growth of ultra-thin films on conventional ferroelectrics as oxide substrates. They exhibit metal-insulator (MI) transition, which could be continuously controlled by composition, bi-axial strain and or electric field. Theoretical description of this class of strongly correlated materials is quite challenging: an ab initio results within DFT+U scheme fail to reproduce correct magnetic ground state, as well as the effect of epitaxial strain on MI transition temperature [1]. In present study we show correlation between MI transition temperature and structural parameters of bulk and films, which agrees well with the existing experimental data. We analyze the difference in the electronic structure obtained within DFT+U and hybrid functionals and the resulting ground state magnetic ordering. We discuss the obtained changes in the electronic structure of bulk materials and strained films and their correlation with experimental MI transition temperatures.

**METHOD**

We present results of our comprehensive study of structural, magnetic and electronic properties of bulk RENiO₃ (RE=Y, Gd, Eu, Sm, Nd and Pr) and strained SmNiO₃ films [2], performed within HSE06 functional [3]. The f shells of RE were treated in core. 80-atomic unit cell was used to account superimposed 2×1×2 magnetic structure. No symmetry constraints were imposed. For structural relaxation we have used projector augmented-wave pseudopotentials as implemented in Vienna Ab Initio Simulation Package (VASP) [4]. The ion positions were relaxed until Hellmann-Feynman forces were smaller than 0.04 eV/Å. GGA+U calculations were performed for different values of U ranging from 1.2 to 9 eV and $J_H=1.0$ eV.

**MOTIVATION**

Ability of switching between metallic and insulating states by external factors is a very demanding property for industrial applications such as ferroelectric memories. In this sense, rare-earth nickelates are very promising materials due to their perovskite crystalline structure, which allows epitaxial growth of ultra-thin films on conventional ferroelectrics as oxide substrates. They exhibit metal-insulator (MI) transition, which could be continuously controlled by composition, bi-axial strain and or electric field. Theoretical description of this class of strongly correlated materials is quite challenging: an ab initio results within DFT+U scheme fail to reproduce correct magnetic ground state, as well as the effect of epitaxial strain on MI transition temperature [1]. In present study we show correlation between MI transition temperature and structural parameters of bulk and films, which agrees well with the existing experimental data. We analyze the difference in the electronic structure obtained within DFT+U and hybrid functionals and the resulting ground state magnetic ordering. We discuss the obtained changes in the electronic structure of bulk materials and strained films and their correlation with experimental MI transition temperatures.

**METHOD**

We present results of our comprehensive study of structural, magnetic and electronic properties of bulk RENiO₃ (RE=Y, Gd, Eu, Sm, Nd and Pr) and strained SmNiO₃ films [2], performed within HSE06 functional [3]. The f shells of RE were treated in core. 80-atomic unit cell was used to account superimposed 2×1×2 magnetic structure. No symmetry constraints were imposed. For structural relaxation we have used projector augmented-wave pseudopotentials as implemented in Vienna Ab Initio Simulation Package (VASP) [4]. The ion positions were relaxed until Hellmann-Feynman forces were smaller than 0.04 eV/Å. GGA+U calculations were performed for different values of U ranging from 1.2 to 9 eV and $J_H=1.0$ eV.

**MOTIVATION**

Ability of switching between metallic and insulating states by external factors is a very demanding property for industrial applications such as ferroelectric memories. In this sense, rare-earth nickelates are very promising materials due to their perovskite crystalline structure, which allows epitaxial growth of ultra-thin films on conventional ferroelectrics as oxide substrates. They exhibit metal-insulator (MI) transition, which could be continuously controlled by composition, bi-axial strain and or electric field. Theoretical description of this class of strongly correlated materials is quite challenging: an ab initio results within DFT+U scheme fail to reproduce correct magnetic ground state, as well as the effect of epitaxial strain on MI transition temperature [1]. In present study we show correlation between MI transition temperature and structural parameters of bulk and films, which agrees well with the existing experimental data. We analyze the difference in the electronic structure obtained within DFT+U and hybrid functionals and the resulting ground state magnetic ordering. We discuss the obtained changes in the electronic structure of bulk materials and strained films and their correlation with experimental MI transition temperatures.

**METHOD**

We present results of our comprehensive study of structural, magnetic and electronic properties of bulk RENiO₃ (RE=Y, Gd, Eu, Sm, Nd and Pr) and strained SmNiO₃ films [2], performed within HSE06 functional [3]. The f shells of RE were treated in core. 80-atomic unit cell was used to account superimposed 2×1×2 magnetic structure. No symmetry constraints were imposed. For structural relaxation we have used projector augmented-wave pseudopotentials as implemented in Vienna Ab Initio Simulation Package (VASP) [4]. The ion positions were relaxed until Hellmann-Feynman forces were smaller than 0.04 eV/Å. GGA+U calculations were performed for different values of U ranging from 1.2 to 9 eV and $J_H=1.0$ eV.

**MOTIVATION**

Ability of switching between metallic and insulating states by external factors is a very demanding property for industrial applications such as ferroelectric memories. In this sense, rare-earth nickelates are very promising materials due to their perovskite crystalline structure, which allows epitaxial growth of ultra-thin films on conventional ferroelectrics as oxide substrates. They exhibit metal-insulator (MI) transition, which could be continuously controlled by composition, bi-axial strain and or electric field. Theoretical description of this class of strongly correlated materials is quite challenging: an ab initio results within DFT+U scheme fail to reproduce correct magnetic ground state, as well as the effect of epitaxial strain on MI transition temperature [1]. In present study we show correlation between MI transition temperature and structural parameters of bulk and films, which agrees well with the existing experimental data. We analyze the difference in the electronic structure obtained within DFT+U and hybrid functionals and the resulting ground state magnetic ordering. We discuss the obtained changes in the electronic structure of bulk materials and strained films and their correlation with experimental MI transition temperatures.

**METHOD**

We present results of our comprehensive study of structural, magnetic and electronic properties of bulk RENiO₃ (RE=Y, Gd, Eu, Sm, Nd and Pr) and strained SmNiO₃ films [2], performed within HSE06 functional [3]. The f shells of RE were treated in core. 80-atomic unit cell was used to account superimposed 2×1×2 magnetic structure. No symmetry constraints were imposed. For structural relaxation we have used projector augmented-wave pseudopotentials as implemented in Vienna Ab Initio Simulation Package (VASP) [4]. The ion positions were relaxed until Hellmann-Feynman forces were smaller than 0.04 eV/Å. GGA+U calculations were performed for different values of U ranging from 1.2 to 9 eV and $J_H=1.0$ eV.