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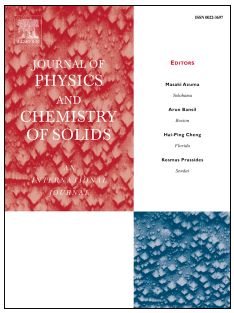

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Electronic and magnetic properties of new half-metallic ferromagnetic rutile $Ti_{1-x-y}V_xNi_yO_2$ ($x = y = 6.25\%$): A first-principles study

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ABSTRACT

We report electronic and magnetic properties of the new half-metallic ferromagnetic co-doped system of rutile $Ti_{1-x-y}V_xNi_yO_2$ ($x = y = 6.25\%$). The semiconductor ferromagnetic doped system of rutile $Ti_{1-x}V_xO_2$ ($x = 6.25\%$) system is revisited as the reference. The plane-wave GGA + U method was used after choosing U at Ti 3d site in the fully-optimized rutile TiO_2. The co-doped system exhibits the total magnetic moment of 1.41 μ_B/Ni atom localized at the V and Ni sites which is significantly higher than that of the doped system. Interestingly, the local ferrimagnetism centered at the cations of V^{4+} and Ni^{3+} is found with the minor contribution from their nearest-neighboring O^{2-} ions bound via the p-d hybridization. The Ni^{3+} ion induces the half-metallic behavior by introducing spin-up hole O 2p states above the Fermi energy level. Finally, the GGA + U provides accurate energy positions of sub-V 3d and Ni 3d states under the elongation Jahn-Teller distortion at the VO_6 and NiO_6 octahedra. Our result shows the significant effect of Ni^{3+} ion in modifying the electronic and magnetic properties of the rutile $Ti_{1-x}V_xO_2$ system. This study presents the essentials properties which can be a guide for experiments.

Keywords: electronic properties; magnetic properties; rutile TiO_2; half-metallic ferromagnetic