

Mn₃O₄ のスピネル相およびポストスピネル相の電子構造Electronic structure of Mn₃O₄ spinel and postspinelHPSTAR¹, 慶応大物情² ○平井慈人¹, 後藤陽介², 神原陽一², 的場正憲²HPSTAR¹, Keio Univ.² ○Shigeto Hirai¹, Yosuke Goto², Yoichi Kamihara², Masanori Matoba²

Manganese oxides have been exploited for a wide range of technological applications including energy storage devices. Mn₃O₄ is a unique mixed-valence oxide that adopts a tetragonally distorted spinel structure at ambient conditions [1]. This phase undergoes a structural phase transition at 15 GPa into a CaMn₂O₄-type phase, referred to as postspinel, which is quenchable to ambient pressure [2]. Mn₃O₄ spinel exhibits pronounced magnetodielectric and magnetoelastic coupling [3]. Mn₃O₄ postspinel undergoes a giant atomic displacement near its T_N (=210 K) due to the coupled effect of the metastable structure with the orbital realignment of the Mn³⁺ ion [2].

Both of these phases are magnetically frustrated [2,3], providing an important playground for systematically studying the electronic band structures of spin frustrated magnets. Previous studies on the band structure of Mn₃O₄ spinel are limited to theoretical studies and no optical studies have been reported for bulk samples of Mn₃O₄ spinel or postspinel.

In this talk, we demonstrate the electronic structure of Mn₃O₄ spinel and postspinel by *ab initio* calculations and the optical absorption spectra. Mn₃O₄ possesses characteristic band-splitting of the conduction band (Fig.1). Both phases of Mn₃O₄ are charge-transfer type insulators, and Mn 3d t_{2g} and O 2p form antibonding orbitals situated at the conduction band with higher energy.

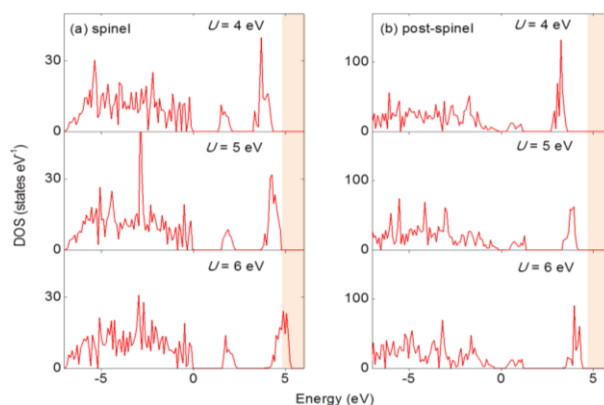


Figure 1. Densities of states in Mn₃O₄ spinel and postspinel calculated in PBE+U method.

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[2] S. Hirai, A.M. dos Santos, M.C. Shapiro, J.J. Molaison, N. Pradhan, M. Guthrie, C.A. Tulk, I.R. Fisher, and W.L. Mao, Phys. Rev. B **87**, 014417 (2013).

[3] T. Suzuki and T. Katsufuji, Phys. Rev. B **77**, 220402 (2008).