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Electronic structure of LaMO$_3$ (M=Ti∼Cu) by GW approximation YOSHIRO NOHARA, TAKEO FUJIWARA, University of Tokyo — We investigate the electronic structure of LaMO$_3$ (M =Ti∼Cu) by GW approximation. The calculated spectra show good agreement with the experimentally observed ones. The on-site Coulomb interaction are affected by strong screening mechanism in trivalent transition metal ion systems, which is qualitatively different from those in monooxides MO of divalent transition metals. In trivalent transition metal ion systems LaMO$_3$, 3d electrons are affected by deep atomic potential. Therefore, the 3d orbital locates energetically much nearer to O 2p levels than in MO. Moreover, in the cases of M^{3+}=Cr^{3+}, Mn^{3+} and Fe^{3+} systems, transition metal ions are well spin-polarized, and 3d levels locate very near to O 2p levels. As a result, these systems have large screening effects due to the extended d-electrons. In the cases of M^{3+}=Ni^{3+} and Cu^{3+}, the systems are metallic and are affected by strong screening effects. In the other cases of M^{3+}= Ti^{3+}, V^{3+}, and Co^{3+}, there are small screening effects causing large static screened Coulomb interaction.

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