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Magnetic properties of $d-$atomic systems with unquenched orbital moments VICTOR ANTONOV, (1). Ames Laboratory USDOE, Ames, IA 50011 (2). Institute for Metal Physics, 36 Vernadsky blrd., Kiev, Ukraine, 03680, LIQIN KE, ANTON JESCHE, VLADIMIR ANTROPOV, Ames Laboratory USDOE, Ames, IA 50011 — Many systems of d-atoms with unquenched orbital moments demonstrate unusually large values of atomic magnetic moments, high magnetic anisotropy and small magnetic ordering temperatures. Using electronic structure analysis, we study a mechanism of the formation of strong on-site electronic correlations that lead to a strong orbital polarization, and in turn, generate a highly orbitally polarized hybridization with non-magnetic host atoms. In this case, even a small spin orbital coupling of $3d$-atoms can create a significant effect. We introduce a consistent model of the formation of large orbital moments and magnetic anisotropy both in the metallic and insulating cases, and apply it to several realistic systems. Detailed calculations of magnetic properties, including magneto-optical studies of the Kerr angle rotation, are performed for several nitrometalates of Mn, Fe and Co where a rather large (3-5 degrees) Kerr angle rotation is predicted for the first time. We further discuss the nature of critical temperature in magnetic phase transition in such systems and the opportunity to increase it.

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