Abstract Title: First-principles electronic and magnetic structures of BiMn2O5, GdMn2O5 and ErMn2O5 under pressure
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Abstract: A large body of research work has been devoted to the study of RMn2O5 magnetoelectrics, where R stands for Bi, Y or a rare earth ion. These compounds are characterized by complex crystal and magnetic structures, as well as a wealth of entangled magnetic and ferroelectric phase transitions [1,2]. In this study we present results of full relativistic GGA+U calculations performed on BiMn2O5, GdMn2O5 and ErMn2O5 compounds under applied pressure, aiming to reveal the changes in the spin and orbital magnetism and to relate them to the electronic structure evolution and local environment distortion.

References [1] J. van den Brink and D. Khomskii, J. Phys.: Condens. Matter 20, 434217 (2008). [2] T. Kimura et al., Ferroelectrics, 354, 77 (2007).