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Spin density distribution in systems with frustrated triangular magnetic structure[1] PAVEL LUKASHEV, RENAT SABIRIANOV, University of Nebraska at Omaha — We present results of ab-initio calculations for the non-collinear spin density (SD) distribution in the systems with frustrated triangular magnetic structure (Mn-based antiperovskites, Mn_3AN (A=Ga, Zn)) in the ground state and under external mechanical strain. We show that SD in the (111)-plane of the unit cell (in particular, in the atomic sphere around Mn atom) is distinctly non-uniform, i.e. both direction and magnitude of SD strongly depend on the distance from Mn site within atomic sphere. We show that the evolution of SD under external mechanical stress exhibits more diverse features than expected in the rigid spin model. In particular, under applied strain we observe the appearance of spin "domains" in the (111)-plane of the unit cell in which SD rotates in opposite directions. The rotation of SD reverses if tensile strain changes to compressive, but the shape of the "domains" stays somewhat stable. We have shown that the change in SD distribution under strain depends on the interplay of exchange interactions governing the rotation of SD in the localized high SD region and the structure of SD in the highly inhomogeneous vortex structure in the interstitial region.

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