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First-principles simulation and low-energy effective modeling of three-dimensional skyrmion in MnGe[1] HONGCHUL CHOI, YUAN-YEN TAI, JIAN-XIN ZHU, Los Alamos National Laboratory, T-4 TEAM — The skyrmion spin textures are mostly observed in two-dimensional (2D) space, which can be topologically mapped onto the surface of the sphere with an integer multiple of topological winding number. Recently, MnGe has been reported as a candidate of 3D skyrmion crystal, showingthe variationof the skyrmion size along the z-direction [1,2]. We have performed the first-principles simulation and constructed a tight-binding model with calculated electronic-structure information to investigate the 3D skyrmion phase in MnGe. Our first-principles study within density functional theory shows that the calculated magnetic moment is larger than that for MnSi (with different lattice constant), implying the possibility of a multiple magnetic transition under pressure [3].We have also found that the small-sized skyrmion could be stabilized in a 2D structure. Such a high density of the skyrmion is in good agreement withthe experimental finding of large topological Hall effect [1]. Finally, we will extend our study to consider the 3D skyrmion structure based on the constructed tight-binding model. [1] Y. Shiomi et al., Phys. Rev. B 88, 064409 (2013); [2] T. Tanigaki et al., Nano Lett. 15, 5438 (2015); [3] M. Deutsch et al., Phys. Rev. B 89, 180407 (2014).

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