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First-principles simulations and low-energy effective modeling of skyrmion in MnGe HONGCHUL CHOI, YUAN-YEN TAI, JIAN-XIN ZHU, Los Alamos National Laboratory — MnGe has been reported as a candidate of three-dimensional (3D) skyrmion crystal, showing the variation of the skyrmion size along the z-direction [1,2]. Also, the small size (3nm) and high density of the skyrmion are the desired properties for information storage. We have performed the first-principles simulations and constructed a tight-binding (TB) model with calculated electronic-structure information to investigate the skyrmion phase in MnGe. Our first-principles study within density functional theory (DFT) shows that the small-sized skyrmion could be stabilized in a 2D structure. Such a high density of the skyrmion is in good agreement with the experimental finding of large topological Hall effect [1]. Using the TB simulation package [3] based on the DFT bandstructure, we have studied skyrmion state in a large supercell of MnGe beyond the DFT capability. The role of the correlation effect and the pinning effect of vacancy have been investigated. Finally, the nature of 3D skyrmion in MnGe has also been discussed. [1] Y. Shiomi et al., Phys. Rev. B 88, 064409 (2013); [2] T. Tanigaki et al., Nano Lett. 15, 5438 (2015); [3] Yuan-Yen Tai and Jian-Xin Zhu, arXiv:1603.03107 (2016)

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