

Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

A First Principles Study of the Large Anomalous Hall Effect in Noncollinear Antiferromagnets Mn_3Ge and Mn_3Sn TZUCHENG WANG, Department of Physics, National Taiwan University, GUANGYU GUO, Department of Physics, National Taiwan University, Physics Division, National Center for Theoretical Sciences, QIAN NIU, Department of Physics, University of Texas — Anomalous Hall effect (AHE) has been thought to be present only in ferromagnetic conductors, with its size being proportional to the net magnetization. Using symmetry arguments and first principles calculations, physicists recently demonstrated that large AHE may appear in noncollinear antiferromagnets [1]. Indeed, the AHE has been recently observed in the spin liquids and antiferromagnets [2,3]. Mn_3Ge and Mn_3Sn are hexagonal chiral antiferromagnets with zero net magnetization which yet exhibit the large AHE being in the same order as in ferromagnets such as Fe [2,3]. Here we calculate the electronic and magnetic structure of Mn_3Ge and Mn_3Sn based on the density functional theory with the generalized gradient approximation. The anomalous hall conductivity of Mn_3Ge and Mn_3Sn are also calculated using efficient Wannier function interpolation. A microscopic understanding of such spin-related transports as AHE in noncollinear antiferromagnets could accelerate development of spintronics.

[1] Chen H, Niu Q and MacDonald A H *Phys. Rev. Lett.* 112 017205 (2014)

[2] Nakatsuji S, Kiyohara N and Higo T *Nature* 527 2125 (2015)

[3] Kiyohara N, Tomita T and Nakatsuji S *Phys. Rev. Appl.* 5 064009 (2016)

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Date submitted: 11 Nov 2016

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