Ab-initio study of magnon in $L1_0$ Mn-based antiferromagnets

Mie Univ., °Koki Kobayashi, Andi Gumarilang, Kenji Nawa, Kohji Nakamura

E-mail: 424M214@m.mie-u.ac.jp

Ultra-fast spin operations in terahertz (THz) frequency range have been demand for future communication technologies. Antiferromagnets are promising candidates to convey this frequency due to no-net magnetization while exhibiting antiferromagnetic resonance in THz range [1], and magnon in antiferromagnets may offer new energy-efficient spin memory technique via their multiple precession modes [2]. Among the antiferromagnetic (AFM) materials, $L1_0$ Mn-based antiferromagnets, such as MnNi, MnPd, and MnPt, have particular attention. Its unique magnetic properties, including the high exchange fields as manifested in high Curie temperature [3], make it suitable for spintronics devices. However, to fully utilize them for spintronics devices, it is essential to understand its fundamental magnetic characteristics related to magnon dispersion. Here, we carry out ab-initio calculations of magnons in $L1_0$ Mn-based antiferromagnets of MnNi, MnPd, and MnPt. Ab-initio calculations were performed using full-potential linearized augmented plane-wave (FLAPW) method [4] with generalized gradient approximation (GGA). The spin-exchange constants are evaluated by applying the generalized Bloch theorem in spin spiral calculations, while the magnetic anisotropy constants are obtained by the force theorem to spin-orbit coupling (SOC) and magnetic dipole-dipole interaction (MDI) approximation. The magnon dispersions are obtained by using second-quantization formalism based on the linear spin wave theory (LSWT) [5]. The first five nearest-neighbors spin-exchange constants, labeled as J_1, J_2, J_3, J_4, and J_5, are calculated for Mn-based antiferromagnets. For MnNi, the values are -86.367, 42.870, 14.412, -3.093, -0.122 meV, respectively. For MnPd these are -50.900, 41.670, 8.766, -4.216, -3.460 meV, and for MnPt, -61.812, 41.606, 6.754, -7.061, -10.509 meV, respectively. The magnon frequency of α mode at Γ are found to be 11.831 THz, 9.732 THz, and 10.416 THz for MnNi, MnPd, and MnPt, respectively, while that of β mode is 1.965 THz, 1.438 THz, and 1.548 THz for MnNi, MnPd, and MnPt, respectively. Based on the density of states, the trend of spin-exchange constants from MnNi to MnPt originates from the energy gap between the highest occupied d-orbital of Mn and the lowest unoccupied d-orbital of Mn, where MnNi has the lowest gap which allows electrons to excite easily than that in MnPd and MnPt.

[1] T. Moriyama *et al.*, Phys. Rev. Mater. **3**, 051402 (2019)

[2] Y. Shiota, *et al.*, Nat Commun **15**, 9750 (2024).

[3] E. Krén, et al. Phys. Rev. **171**, 574 (1968).

[4] K. Nakamura, *et al.*, Phys. Rev. B **67**, 014420 (2003).

[5] A. Gumarilang, *et al.*, J. Phys. Soc. Jpn, **92**, 084703 (2023).