First-principles study of magnon dispersion and magneto-optical Kerr effect of antiferromagnetic L10-type MnPt

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Antiferromagnetic (AFM) materials are attracting attention due to weak response to external magnetic fields and fast spin dynamics in the THz frequency range. In particular, high Néel temperature AFM materials may be great candidates for future spintronic devices. We use first-principles calculations based on density functional theory and the spin spiral approximation to study the magnon dispersion of AFM L10-type MnPt. Néel temperatures computed using the mean-field/random-phase approximation are 1.12%/20.9% smaller than experimental results. For studying the magneto-optical Kerr effect (MOKE), a fully relativistic band structure and dielectric tensor are computed. We simulate the change of the MOKE signal under magnetization on the order of 3.98µB per unit cell by spin flipping and tilting. Kerr rotation angles increase linearly with magnetization, corresponding to spin tilting, while there is no signal without spin tilting due to compensating AFM spin configuration. Our results show that Kerr rotation is three times larger in the UV region than for visible light.