First principles calculations of magneto-optical conductivity in heavy metals

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An interest of spin-polarized electrons playing a central role in spintronics has been growing in optoelectronic applications using circularly polarized light. At an earlier stage in this field, an attention was paid to a spin-polarized electron emission from semiconductor heterostructures [1], e.g., by using a strained GaAs thin-layer that leads to exited electrons with highly spin-polarization as much as 86% [2]. It is however demanded more efficient materials for the photo-spin current conversion in the applications. Although first-principles calculation is known to be an effective tool to search such materials, there is no report available. In the present work, the magneto-optical conductivity to spin currents for 5d heavy metals, as well as GaAs, were investigated in order to search the material candidates. Self-consistent calculations were carried out by using full-potential linearized augmented plane-wave method [3] based on the generalized gradient approximation, and the conductivity coefficients as a function of photo energy were evaluated on the basis of Kubo-formula in the linear response theory by using the calculated eigenvectors. For GaAs, we observe the off-diagonal component of the magneto-optical conductivity, reflecting the excited spin-polarized electrons by circularly polarized light even though the spin-orbit-coupling (SOC) of GaAs is weak, which agrees with experiments. For 5d heavy metals, we find that the intensity significantly increases due to the large SOC, for example, for Pt the intensity ranging from 1 eV to 2 eV of photo energy increases by one order of magnitude compared to that of GaAs. More details including the mechanism will be presented.