

# Magneto-Optical Properties for Spintronics Materials from First Principles

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The magneto-optical (MO) effects such as Kerr effect, Faraday effect, and the X-ray magnetic circular dichroism, are direct consequences of the dependence of optical conductivity tensor on the magnetic state and can be traced back to different interaction of left- and right- circularly polarized lights with the magnetic solid. MO measurements are therefore powerful experimental probe that play an important role in clarifying the electronic structures of ferromagnets. Within the fascinating field of Spintronics where the electronic structures as well as the magnetic properties of the materials are crucially needed to be elucidated, the MO effects are known to be highly useful to provide detailed information of the material. Here, we present our recent results on the first-principles calculations of the MO effects using the DFT-FLAPW [1] method for three typical Spintronics materials which are the Ga(1-x)Mn(x)As alloys in the pure and defective forms, the Co-based full Heusler alloys, and Ge(1-x)Mn(x) alloys [2,3,4].

In our approach based on the local spin density approximation to the density functional theory, the Kohn-Sham equations are solved self-consistently within the generalized gradient approximation while the Spin-orbit coupling (SOC), essential to describe MO, is treated in the second variational way. The optical conductivity tensor is evaluated from the Kubo formalism within the linear response theory by implementing the Kohn-Sham eigenvalues and eigenfunctions for the interband transitions. Contribution from the intraband transition is added to the diagonal component of the conductivity tensor with the phenomenological Drude expression.

From our calculational results on the Ga(1-x)Mn(x)As in the pure and defective alloys, it is found that (i) the Kerr factor shows a marked minimum occurring at a phonon energy of  $\sim 1.5$  eV while not strongly affected by the Mn concentration for the intermediately dilute range of 6~12% substitutional doping and (ii) for interstitial Mn, the calculated MO results exhibit a significant difference with the substitutional Mn and bear a striking resemblance to the experimental spectra, pointing to the comparison between simulated and experimental Kerr angles as a valid tool to distinguish different defect types in the dilute magnetic semiconductors. Also the Co-based full Heusler alloys, that is, Co<sub>2</sub>MnGe and Co<sub>2</sub>MnSb are studied to reveal that (i) the first low energy minimum is mostly due to optical contributions whereas the second peak shows the magneto-optical origin and (ii) a better agreement with experimental results can be achieved by taking into account of the exact measurement conditions such as the multi-layered

structure by substrate. On the other hand, the X-ray absorption is calculated and compared to the experimental XAS spectra measured for the ion-implanted Ge(1-x)Mn(x) alloys and finds that, while the nature of semiconducting host is shown to affect only slightly the Mn absorption spectrum, the homogeneity of Mn dilution can be effectively recognized by comparing the Mn spectra in dilute MnGe alloys with other competing Mn-Ge crystalline phases. These results demonstrate that the first principles MO calculations are able to identify the features of experimental spectra in terms of spin- and band- resolved electronic transitions and thus, upon combining with experimental investigations, constitute a powerful approach in designing new materials.

#### References

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