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Frist-Principles Study of Magnetic Susceptibility and Field-Dependent Magneto-Optics in Antiferromagnetic Materials

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1 Introduction

A magnetic field has been popularly exploited in experiments to manipulate the magnetic properties of materials. The material's response under the external magnetic field can be quantified by magnetic susceptibility. In the computational approach, the magnetic susceptibility is evaluated in the limit of atomistic spin dynamics level, preventing studies on field-dependent quantum mechanical properties [1]. Therefore, the demand for the prediction of magnetic susceptibility and field-dependent phenomena from first-principles methods increases.

2 Methodology [2]

In a new approach, we use the tilting behavior of magnetic moments under the external field. The total energy change with moment-tilted states in density functional theory calculations naturally includes complex spin-spin interactions, such as exchange interactions. By adding the Zeeman energy term, we can find the lowest total energy state under a certain magnetic field, allowing us to extract corresponding net magnetization. At last, magnetic susceptibility can be evaluated by a magnetic field and extracted net magnetization. Materials with two magnetic sites require two tilting angle dimensions to evaluate the lowest total energy state under the field.

3 Results [2]

Fig. 1 shows the comparison between calculated and measured magnetic susceptibility of antiferromagnetic materials, showing reasonably good agreement. We found that the calculated magnetic susceptibility of M2As (M = Cr, Mn, Fe) and Mn3Sn present some discrepancy, which turned out that the measured results don't follow the typical temperature-dependent behavior of magnetic susceptibility in antiferromagnets. This might be caused by off-stoichiometry or paramagnetic defects. One of the benefits of the new approach is the possibility of field-dependent property calculations. Fig. 2 displays the generation of the polar magneto-optical Kerr effect caused by the external magnetic field. The magneto-optical signal increases with the strength of the magnetic field. Therefore, it demonstrates that a new approach might be used to investigate various field-dependent properties.

4 References

[1] O. Erikssson, A. Bergman, L. Bergqvist, J. Hellsvik. Atomistic spin Dynamics (Oxford University Press, 2017)

[2] K. Kang, K. Yang, K. Puthalath, D. G. Cahill, A. Schleife Phys. Rev. B 105, 184404 (2022)

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