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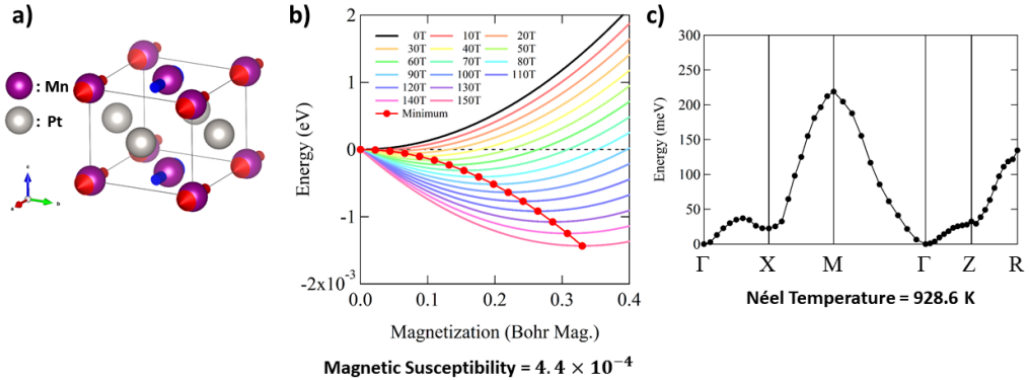
MAGNETO-OPTICAL KERR EFECT OF ANTIFERROMAGNETIC MATERIALS IN EXTERNAL MAGNETIC FIELDS



(a) Magnetic unit cell of MnPt; (b) magnetization and energy change of MnPt spin-tilted calculation for corresponding external magnetic fields. Red marker line in (b) presents ground states under corresponding fields and (c) magnon dispersion of MnPt.

Research Challenge

Antiferromagnetic materials have interesting properties that can potentially lead to fast switching in future memory devices. Spin compensation makes detecting the spin information of antiferromagnetic materials using optical measurements challenging. Measurements of optical response under external magnetic fields have been developed; however, it is still necessary to understand the fundamental behavior of antiferromagnetic materials better. In order to understand basic principles experiments can benefit from detailed theoretical calculations.

Methods & Codes

The Vienna Ab-Initio Simulation Package (VASP) was used for first-principles calculations based on density functional theory to understand the magnetic properties of antiferromagnetic materials. Relaxations of experimental structures were performed in the presence of magnetism and the resulting structures used to compute MOKE signals and Néel temperatures.

Results & Impact

In this project, wavelength-dependent MOKE spectra are computed for MnPt and Fe_2As. The results of magnetic susceptibility and Néel temperature calculations illustrate that this first-principles computational approach can provide reasonable predictions for magnetic properties of antiferromagnetic materials. Thus, our calculations are helpful guidance to understand the behavior of antiferromagnetic materials and to develop advanced magnetic devices.

Why Blue Waters

Computing fully relativistic band structure and its dielectric function with magnetism are demanding processes. Spin-tilted calculations are challenging because noncollinear calculations need more computational resources than collinear calculations. Blue Waters is well suited due to its fast communication and large amount of memory per node and thus provides a unique chance to unveil the unknown properties of antiferromagnetic materials.