Light-Induced and Strain-Tunable Magnetic Control in Layered Mn-Pnictides

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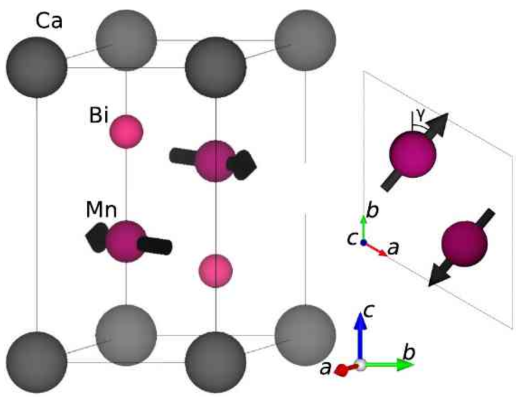
Understanding the dynamic control of magnetism in layered materials is essential for advancing next-generation spintronic and optoelectronic applications. Recent experiments on the magnetization dynamics of the layered narrow-gap antiferromagnet $CaMn_2Bi_2$ show evidence of a magnetic reorientation transition induced by above-gap optical excitation [1]. The light-induced magnetization reorientation can occur here due to strong magnetoelastic coupling, which brings the system out of equilibrium and allows ultrafast spin-state control. The large coupling between light and magnetic order in this material also suggests that related phenomena could be accessed via additional tuning parameters like strain. In fact, we note that a key ingredient is the interplay between spin-orbit coupling (SOC) and lattice distortions. Using first-principles calculations within density functional theory (DFT) with Hubbard corrections and SOC, we study the role of strain in tuning magnetic anisotropy and find that small strain values induce a transition between in-plane and out-of-plane magnetization states. Furthermore, our calculations extends the Heisenberg model to include an on-site magnetization term, which accurately capture magnetic excitations beyond simple exchange interactions. These results showed Mn-based honeycomb materials as promising candidates for controllable 2D magnetic systems, and paves the way for ultrafast, strain-engineered spintronic and magnetooptical applications.

References

[1] BT Fichera, B Lv, K Morey, Z Shen, C Lee, E Donoway, A Liebman-Peláez, A Kogar, T Kurumaji, M Rodriguez-Vega, RH Aguilera-del-Toro, M Arruabarrena, B Ilyas, T Luo, P Müeller, A Leonardo, A Ayuela, GA Fiete, JG Checkelsky, J Orenstein, and N Gedik, Physical Review X (accepted).

[2] RH Aguilera-del-Toro, M Arruabarrena, A Leonardo, M Rodriguez-Vega, GA Fiete, A Ayuela, arXiv:2410.23053

Figures



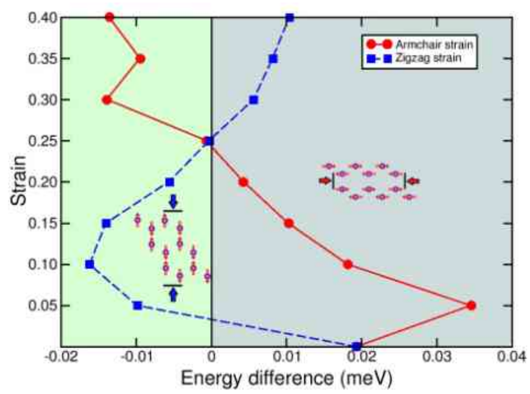


Figure 1: (a) Magnetic unit cell of CaMn2 Bi 2. The angle γ is such that the Mn spin does not lie precisely along any particular crystallographic axis. (b) In-plane magnetic anisotropy energy difference when the strain is applied along the two main hexagonal directions. The blue region indicates that the zigzag direction is preferred; the green region indicates that the armchair direction is preferred.