

First-Principles Study of Strain-Controlled Magnetism in MnBi_2Se_4 Heterostructures

We present a first-principles study of the magnetic ground state of the quantum magnetic material MnBi_2Se_4 supported on a ferroelectric substrate. Using density functional theory, we first compare competing ferromagnetic and antiferromagnetic configurations of freestanding MnBi_2Se_4 . We then construct a fully relaxed MnBi_2Se_4 /ferroelectric heterostructure and determine its equilibrium geometry and magnetic ground state. Finally, shear strain is applied to the relaxed heterostructure to investigate its effect on the relative stability of competing magnetic configurations. We find that shear strain produces a non-monotonic evolution of the magnetic ground state, driving transitions among ferromagnetic, zigzag-antiferromagnetic, and stripy-antiferromagnetic states over the investigated strain range. These results demonstrate that mechanical deformation can provide an effective means of controlling magnetism in MnBi_2Se_4 -based ferroelectric heterostructures. Our findings highlight strain engineering as a promising approach for manipulating magnetic states in low-dimensional quantum materials, with potential implications for spintronic applications.