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First-principles study of magnetic ion doping in thin film Bi_2Se_3: electronic structure and topological phase[1] JINO IM, HOSUB JIN, ARTHUR J. FREEMAN, Northwestern University — We study the quantum anomalous Hall state in magnetic ion-doped Bi_2Se_3 thin films. By using first-principles density functional theory, we investigate this electronic structure and identify its topological phase. We find that magnetic ion doping induces the exchange field splitting and changes the spin-orbit coupling strength. As the doping concentration increases, the exchange field splitting strength increases and the spin-orbit coupling strength may decrease depending on the type of magnetic ion. Based on these results, we show that the quantum anomalous Hall state in the doped Bi_2Se_3 thin film emerges at a certain range of doping concentration. The Hall conductance of the doped Bi_2Se_3 thin film will also be discussed with various doping concentrations.

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