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Codoping-enhanced magnetism in 4f transition metal doped Bi₂Se₃¹ JUNYI ZHU, BEI DENG, YIOU ZHANG, Chinese University of Hong Kong, SHENGBAI ZHANG, RPI, YAYU WANG, KE HE, Tsinghua University — Despite the great success in the realization of the quantum anomalous Hall effect (QAHE), it was only observed at extremely low temperatures due to the low ferromagnetic Curie temperature and the tiny magnetically induced gap. To fully understand the mechanism of the ferromagnetic ordering, thereby improving the ferromagnetism, we investigated 4f transition metal doped Bi₂Se₃, using density functional theory approaches. We predict that Eu and Sm can introduce stable long-range ferromagnetic states in Bi₂Se₃, with large magnetic moments and low impurity disorders. Additionally, codoping is proposed to tune the Fermi level into the gap, which simultaneously improves the magnetic moment and the incorporation of magnetic ions. Our findings, thus, offer a new novel strategy in facilitating the realization of QAHE in TI systems.

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