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Magnetic Coupling in $FeBi_2Se_4$ and $FeSb_2Se_4$ from first principles
LOGAN WILLIAMS, EMMANOUIL KIOUPAKIS, JUAN LOPEZ, PIERRE FERDINAND P. POUDEU, University of Michigan — Spintronic devices offer benefits in power efficiency and size reduction over current electronics, but require the development of semiconductor materials with favorable magnetic properties. Specifically, a high ferromagnetic-to-paramagnetic Curie transition temperature is required for spintronics operation at room temperature. $FeBi_2Se_4$ and $FeSb_2Se_4$ are two n and p-type magnetic semiconductors, respectively, with Curie transition temperatures of 450K. We employ first-principles calculations based on density functional theory to examine the magnetic coupling mechanisms in these materials. Our results indicate that antisite defects of Fe upon the Bi/Sb sites are crucial to the ferromagnetic coupling of the Fe magnetic moments in the crystals. This research was supported by the National Science Foundation CAREER award through Grant No. DMR-1254314. Computational Resources were provided by the DOE NERSC facility.

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