CoFeVSb: A Promising Spintronic and Thermoelectric Material

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We present a combined theoretical and experimental study of a novel quaternary Heusler system CoFeVSb from the viewpoint of room temperature spintronics and thermoelectric applications. It crystallizes in cubic structure (space group F-43m) with a small DO_3-type disorder. The crystal structure is confirmed by room temperature synchrotron X-ray diffraction (XRD) and extended X-ray absorption fine structure (EXAFS) measurements. Magnetization data reveal a high ordering temperature (T_C ~850K) and ferromagnetic feature with a saturation magnetization of 2.2 μ_B/f.u. Resistivity measurements indicate half-metallic/semi-metallic nature. Double hysteresis loop along with asymmetry in the magnetoresistance (MR) data reveals room temperature spin-valve feature, which remains stable even at 300 K. Hall measurements show anomalous behavior with significant contribution from intrinsic Berry phase, which is further confirmed by the theoretical calculations. This alloy also has a large room-temperature power factor (~ 0.62 mWatt/m/K^2) and ultralow simulated lattice thermal conductivity (~ 0.4 W/m/K), making it a promising candidate for thermoelectric application. Ab-initio calculations suggest weak spin-polarized semimetallic behavior and reduced magnetization (in agreement with the experiment) in presence of DO_3 disorder. We have also found an energetically competing ferromagnetic (FM)/antiferromagnetic (AFM) interface structure within an otherwise FM matrix; one of the prerequisites for spin-valve behavior. Hard X-ray photoemission spectroscopy (HAXPES) data also validates the semimetallic-like density of states (DoS), which further supports the theoretical findings. The coexistence of so many promising features in a single system is rare, and hence CoFeVSb gives a fertile platform to explore numerous applications in the future.

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