Metallic Antiferromagnetic Spintronics: Mn2Au a Case Study

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Abstract. The band structure of bulk Mn2Au has been investigated by first-principles density-functional theory calculations based on the Green's function technique. The total density of state reveals contributions mainly from the Au5d and Mn3d states with rigid local moments on the Mn sites. The existence of significant out-of-plane magnetic anisotropy combined with the large strength of short range antiferromagnetic exchange interactions between Mn atoms located at two different Wyckoff positions results in the stabilization of the antiferromagnetic ground state. One-step model Angle resolved photoemission calculations of constant energy surfaces in the Γ-X-Σ plane of the Brillouin zone exhibits a 4-fold to 2-fold symmetry breaking as a function of the binding energy at 0.00 eV and 0.25 eV below the Fermi surface. We find that such a symmetry breaking in Mn2Au is arising due to the degeneration of the electronic bands in the presence of external magnetic field indicating a strong spinorbit coupling interaction. Our results describes the tuning of the magnetic and electronic properties of Mn2Au by external magnetic field and chemical doping for spintronic applications.