

Electronic Structure and Angle-Resolved Photoemission Spectra of Antiferromagnetic Mn₂Au(001) within the One-Step Model

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Abstract. Electronic structure of antiferromagnetic Mn₂Au has been studied by utilizing first-principles density-functional theory calculations based on the Green's function technique. The total density of states reveal contributions from the Au4f and two Mn3d states with collinear antiferromagnetic order with localized magnetic moments. Our ground state band structure calculations representing the Bloch spectral functions shows that the essence of the AF-switching induced by Neel spinorbit torques in Mn₂Au is in the Γ X direction indicating a band crossing for Neel vector oriented along [100] direction. The one step model angle resolved photoemission calculations in a Kz band map for photon energies ranging from 400 - 1000 eV shows dispersive spectral weight at Fermi level along Γ Σ direction.