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Noncollinear magnetism at ferromagnetic/antiferromagnetic interfaces: canting and half-metallicity K. NAKAMURA, T. ITO, Mie University, A.J. FREEMAN, Northwestern University — We present first principles determinations of noncollinear magnetic structures at the exchange bias FM/AFM interfaces by using the FLAPW method¹ including intra-atomic noncollinear magnetism² to treat the magnetic complexity at interfaces involved in the spin-flop coupling. First, we demonstrate exchange bias at the Co/FeMn interface, in which we find that the Fe moments in the FeMn layer reorient away from their directions in bulk FeMn so as to be parallel to the Co moment direction, which induces an out-of-plane magnetic anisotropy. The results appear to support and confirm recent experimental XMCD findings that rule out spin-flop coupling as the mechanism for the exchange bias in this system. Next, we determine magnetic structures at the CrSe/MnSe and CrTe/MnTe interfaces, in order to investigate exchange-biased half-metallic ferromagnets. The results show that the Cr moments in the FM layer lie perpendicular to the Mn moments in the AFM layer but that the Mn moments strongly cant to induce net moments at the AFM interfaces. Importantly, we find that the canting of the moments tends to retain the half-metallic state at the FM/AFM interface.

¹Wimmer, Krakauer, Weinert and Freeman, PRB 24, 864(1981) ²Nakamura, Freeman, Wang, Zhong and Fernandez-de-Castro, PRB 65, 12402 (2002); 67, 14420 (2003)

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