Invited Talk, Monday, May 6, 2:00 p.m.-2:40 p.m., ICAMS^2 session: **M2**

Development of a magnetic bond-order potential for Mn phases

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Elemental Mn displays five different phases: the ground-state α-Mn takes the topologically close-packed (TCP) χ-phase (cI58) with β-Mn (cP20), γ-Mn (fcc) and δ-Mn (bcc) stabilised with increasing temperature and ε-Mn (hcp) observed under pressure. Using the DFT binding energy curves for these five phases at T=0K as a database, we have fitted an orthogonal tight-binding (TB) d-band model that qualitatively reproduces the non-magnetic and anti-ferromagnetic DFT curves. Since the magnetic energies are an order of magnitude smaller than those in Fe, the magnetic analytic BOP expansion for Mn requires not 9 but 18 exact moments before converging to the TB results. Interestingly, whereas it is commonly thought that the TCP χ-phase of the Mn ground state is stabilised by size differences between the large and small moment sites, in practice non-magnetic α-Mn is still predicted to be the ground state, so that magnetism is not the critical driving factor. The magnetic moments on the four α-Mn sites are well reproduced. Finally, given the complexity of the non-collinear magnetism (NCLM) that is observed experimentally in α-Mn, we have applied BOP to discuss non-collinear states in the much simpler bcc structure of Fe. The limitations of a purely d-band model are highlighted.