

Abstract Submitted  
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**First-principles study of magnetic properties of Fe-Ni based alloys**<sup>1</sup> M. ONOUE, G. TRIMARCHI, A.J. FREEMAN, Northwestern U., Evanston (IL) — Investigations of the magnetic properties of Fe-Ni based alloys are important from the fundamental as well as technological points of view. Furthermore, the magnetization at saturation and Curie temperature ( $T_C$ ) of FeNi can be tuned for specific applications by alloying with other metallic species. We have performed electronic structure calculations on Fe-Ni- $M$  alloys, where  $M$  are 3d transition metals, to determine how the magnetization depends on the species  $M$  and alloy composition. Electronic band structure and total energies are calculated by the Korringa-Kohn-Rostoker method within the coherent-potential-approximation (KKR-CPA). For the KKR-CPA calculations, we use the generalized gradient approximation of the exchange and correlation functional. In the case of  $\text{Fe}_{0.50}\text{Ni}_{0.45}M_{0.05}$  ( $M=\text{Sc, Ti, V, Cr, Mn, and Co}$ ), the early 3d atoms have antiparallel magnetic moments to the Fe or Ni, whereas the late ones, Mn and Co, have a parallel magnetic moment.

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