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Novel ground states in mixed bcc/fcc, high-/low-spin Fe-(Ni,Pd,Pt) from first-principles[1] SERGEY V. BARABASH[2], ROMAN V. CHEPULSKII[3], VOLKER BLUM[4], ALEX ZUNGER, National Renewable Energy Laboratory, Golden, CO 80401 — Among the observed ordered phases of Fe-X (X=Ni,Pd,Pt), some structures are curiously absent: $L1_2$ Fe_3Pt exists, but Fe_3Pd and Fe_3Ni do not; $L1_0$ FePt and FePd exist, but the stability of $L1_0$ FeNi is debated. Furthermore, the recently measured short range order (SRO) in Fe-rich Fe-Ni is at odds with $L1_2$-type SRO. Theory has been hindered by the appearance of geometric (bcc/fcc) and magnetic (high-spin [HS]/low-spin [LS]) bi-stabilities. We address such bi-stabilities by performing first-principles mixed-basis cluster expansion with added geometric and magnetic "filters," separating structures according to HS/LS and "degree" of fcc-ness and bcc-ness. We performed separate fcc HS and (for Fe-Pd) bcc HS cluster expansions. We predict that *at low temperatures*: (i) New ordered structures exist, including fcc Pt_8Ti-type FeX_8 and the (100) superlattices Fe_2Pd and Fe_2Pt; (ii) *All* fcc Fe_3X compounds are unstable w.r.t. bcc Fe + $L1_0$ FeX (iii) Fcc FePd is unstable w.r.t. bcc Fe + (100) Fe_2Pd superlattice, while $L1_0$ FeNi is, in fact, stable w.r.t. bcc Fe + $L1_2$ $FeNi_3$. At high T, (iv) The SRO in Fe-rich Fe-Ni is governed by (100) superlattice ordering.

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