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Theoretical modeling of epitaxial growth and properties of Mn/Ge (001) multilayers[1] J.E. MEDVEDEVA, A.J. FREEMAN, J.B. KETTERSON, Northwestern University — As part of the search for useful dilute magnetic semiconductors, structural, electronic and magnetic properties of Mn/Ge (001) digital alloys and multilayers are determined using our highly precise full-potential linearized augmented plane wave (FLAPW) method[2]. First, the calculated formation energies of the fully relaxed structures with different Mn and Ge site locations (both substitutional and interstitial), predict the lowest-energy structure in an epitaxial growth process. We found that (i) substitutional positions are energetically more favorable for one (001) monolayer of Mn in the supercell and (ii) when the number of Mn layers increased, the magnetic atoms prefer a second-layer interstitial site and form a 45°-rotated fcc structure on the Ge diamond structure. For the Mn/Ge (001) multilayers, which consist of 8 layers of Ge and 1 or 4 layers of fcc Mn, we found that the experimental ferromagnetic coupling between Mn atoms can be reproduced only when Coulomb interactions are taken into account; indeed, LDA+U estimates of T_c as a function of the Mn layer thickness are in good agreement with experiment[3].

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[2]E.Wimmer, H.Krakauer, M.Weinert, A.J.Freeman, PRB **24**, 864 (1981)
[3]J.J.Lee, J.E.Medvedeva, J.H.Song, Y.Cui, A.J.Freeman, J.B.Ketterson (to be published)

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