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First-principles calculations of adsorption and incorporation of Mn on GaAs-(110) surfaces XUAN LUO, RICHARD MARTIN, University of Illinois at Urbana-Champaign — Using first-principles total-energy methods, we investigate the addition of Mn on the GaAs(110) surface. Our results show that Mn atoms can be adsorbed on GaAs(110) with a preference for the middle site between two Ga atoms along the [001] direction, that is to be adsorbed at the center of triangle formed by two surface As atoms and one surface Ga atom. The calculations show that Mn should be incorporated into the first layer since substitution of the Mn for a Ga atoms results in a larger binding energy. This is in agreement with STM images from our collaborating experimental group[1] and with previous tight-binding calculations[2]. Studies are in progress on complexes of two and more Mn atoms on the surface.

References:
1. See talk by A. R. Richardella, D. Kitchens, and A. Yazdani.
2. H. X. Fu, L. Ye, K. M. Zhang and X. D. Xie, Surface Science, vol. 341 273, (1995).

Xuan Luo
university of Illinois at Urbana-Champaign

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