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First-principles study of alloy formation at Fe/GaAs interfaces
IGOR ZUTIC, STEVEN ERWIN, Center for Computational Materials Science, Naval Research Lab — The combination of the high Curie temperature of Fe, high-quality epitaxial growth of Fe on GaAs, and demonstrated high-efficiency spin injection in GaAs, together make Fe/GaAs heterojunctions very attractive candidates for room-temperature spintronic applications. However, little is known about the structure of Fe/GaAs interfaces, and there is a range of conflicting experimental results describing them—including findings of magnetically dead layers [1], an intermediate FeGaAs phase [2], and bulk-like magnetic moments at the interface [3]. Motivated by these findings, we use density-functional theory to study the structural and magnetic properties of interfaces involving possible alloyed phases occurring between Fe and GaAs. From the calculation of interface formation energies we report results on the stability of various structural and magnetic configurations, and provide microscopic parameters which may be used in studies of spin transport to assess the device potential of these heterostructures. [1] J. J. Krebs, B. T. Jonker, and G. A. Prinz, J. Appl. Phys. 61, 2596 (1987). [2] J. Deputier, R. Guerin, B. Lepine, A. Guivarc'h, and G. Jezequel, J. Alloys Comp. 262, 416 (1997). [3] J. S. Claydon, Y. B. Hu, M. Tselepi, J. A. C. Bland, and G. van der Laan, Phys. Rev. Lett. 93, 037206 (2004).

Igor Zutic
Naval Reserach Lab

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