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**Ab initio Investigation of the Failure of Efficient Spin-Injection  
in Fe/GaAs Superlattices** SINEAD GRIFFIN, NICOLA SPALDIN, ETH Zürich

— Magnetic metal-semiconductor systems have been widely studied for use as spintronic devices. The injection of elemental ferromagnetic Fe into GaAs shows great device potential because of the relatively high Curie temperature of Fe compared to other possible injection materials. However, spin-injection in Fe/GaAs has not been successful with several phases such as FeAs and Fe<sub>2</sub>As forming at the interface. We perform Density Functional Theory calculations on bulk FeAs and Fe<sub>2</sub>As to elucidate the structural and magnetic ground states. We then incorporate these Fe-As layers into GaAs/FeAs superlattices and investigate the resulting structures. Both the effects of Fe content and the number of layers in the heterostructure on the magnetic and electronic properties are considered. Our results show that the magnetic ground state of the FeAs compounds helps to explain the failure of spin-injection in these superlattices.

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