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**Electronic Structure and Schottky Barrier Formation in Fe/GaAs  
Magnetic Junctions**<sup>1</sup> DENIS DEMCHENKO, AMY LIU, Georgetown University

— In the most successful experiments, spin injection efficiencies of 2% at room temperature and 30% at low temperature were achieved [1,2]. The role of intrinsic Schottky barriers in controlling spin-dependent tunneling through the interface is crucial since the barriers significantly reduce the conductivity mismatch, which would otherwise eliminate the possibility of spin injection almost entirely. In this work electronic and magnetic properties of Fe/GaAs magnetic junctions are investigated using the first-principles plane wave based pseudopotential method. It has been shown that the properties of such junctions can differ significantly depending on the interface structure [3]. Therefore, here we calculate wide range of properties of Fe/GaAs junctions, including Schottky barrier heights, magnetization profiles, charge distributions, potential profiles, and equilibrium structures of such junctions, and show how these properties depend on the interface structure. [1] H.J.Zhu et al., Phys. Rev. Lett. **87**, 016601 (2001). [2] A.T.Hanbicki et al., Appl. Phys. Lett. **80**, 1240 (2002). [3] S.C.Erwin et al., Phys. Rev. B **65**, 205422 (2002).

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