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Electronic structure of Fe/MgO and Fe/vacuum interfaces: QSGW theory SERGEY FALEEV, University of Alabama, MINT, OLEG MRYASOV, University of Alabama, Department of Physics — Magnetic tunnel junctions (MTJs) and, in particular, Fe/MgO/Fe MTJ have attracted much attention recently due to discovery of large magneto-resistance. Here we study electronic structure of Fe/MgO and Fe/vacuum interfaces using recently developed Quasiparticle Self-Consistent GW (QSGW) theory [1]. We show that electronic structure of Fe/MgO calculated within the QSGW allows one to resolve the so-called 'zero-bias anomaly' contradiction between experimental results and earlier LDA/DFT predictions for Fe/MgO/Fe MTJs. For Fe/MgO and Fe/vacuum systems the QSGW results are in a good agreement with the tunneling conductance measurements [2], but in contract with earlier LDA/DFT calculations [3,4]. Presented results show that accurate of electronic structure beyond LDA/DFT is necessary to describe correctly transport properties of MgO based MTJs. [1]. S. V. Faleev, M. van Schilfgaarde, and T. Kotani, Phys. Rev. Lett. **93**, 126406 (2004) ; M. van Schilfgaarde, T. Kotani, and S. V. Faleev, , Phys. Rev. Lett. **96**, 226402 (2006). [2]. P.-J. Zermatten, G. Gaudin, G. Maris, M. Miron, A. Schuhl, et.al., Phys. Rev. B **78**, 033301 (2008). [3]. W. H. Butler, X.-G. Zhang, and T. C. Schulthess, and J. M. MacLarenm, Phys. Rev. B **63**, 054416 (2001). [4]. K. D. Belashchenko, J. Velev, and E. Y. Tsymbal, Phys. Rev. B **72**, 140404(R) (2005).

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