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Complex Band Structure of MgO, CaO, SrO, BaO insulators: DFT-LDA vs. QSGW theory OLEG MRYASOV, University of Alabama, Department of Physics, SERGEY FALEEV, University of Alabama, MINT — The recent discovery of a very large magneto-resistance in highly crystalline tunnel junctions with MgO barrier triggered extensive experimental research in the field. The complex band structure of the barrier material is an important property of corresponding MTJs [1]. This property have been studied theoretically on the basis of the density functional theory within the local density functional approximation (DFT-LDA) [1,2]. In this work we compare DFT-LDA and QSGW theory results for lowest evanescent states decay constants for a number of oxides MgO, CaO, SrO, BaO. We employ recently developed QSGW theory [3] to calculate electronic band structure. Then the attenuation constant for evanescent states in the band gap have been calculated by interpolating electron dispersion relation using polynomial fit, procedure analogous to one suggested and tested in [1]. We find that attenuation constant for evanescent states does not simply scales with the value of band gap. [1]. W. H. Butler, X.-G. Zhang, and T. C. Schulthess, and J. M. MacLarenm,Phys. Rev. B **63**, 054416 (2001) [2]. K. D. Belashchenko, J. Velev, and E. Y. Tsymbal, Phys. Rev. B **72**, 140404(R) (2005) [3] M. van Schilfgaarde, T. Kotani, and S. V. Faleev, Phys. Rev. Lett. **96**, 226402 (2006);

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