Magnetic tunnel junctions (MTJ), such as Fe/MgO/Fe, are widely used in modern magnetic sensors (i.e. in read heads of hard disk drives) and have shown great potential for applications in many other emerging magnetic devices. The details of the electronic structure of this highly crystalline MTJs define many properties of the devices, such as magneto-resistance (MR) dependence on the MgO thickness and bias voltage dependence. Examples of important electronic structure features that still are a subject of controversies include the position and role of interface Fe states, alignment of the Fe Fermi energy inside the MgO band gap, the decay constant of evanescent states, etc. Ability to account for these features (more precisely than existing models) may help us to understand better underlying physics and eventually improve device performance.

In present work we used beyond LDA/DFT method – recently developed Quasiparticle self-consistent GW (QSGW) approach that unlike DFT is based on the many-body theory and is shown to describe many properties of different classes of materials better than DFT. In order to demonstrate accuracy of the QSGW method we present on Figure 1 the band gaps of a number of oxides calculated by LDA, QSGW, and so-called ‘scaled’ modification of QSGW method that takes into account electron-hole interactions. One can see that QSGW and, particularly, scaled QSGW accurately describe the band gaps even for such strongly correlated systems as NiO where LDA completely fails.

Modern magnetic sensors operate at small bias voltage of the order of 0.1-0.2 eV. Thus, accurate description of the minority surface states near the Fermi energy (peak at +0.12 eV in DOS) is essential for simulation of real devices. As one can see from Figure 2, the QSGW describes this peak more accurately compare to the LDA. Additionally, the shift of the peak from the Fermi level to +0.12 eV explains why no zero-bias anomaly has been observed experimentally.

Results for Fe(100) surface

Figure 1. Band gaps of oxides calculated by LDA, QSGW and scaled QSGW methods in comparison with experiment. The (highly systematic) deviations of the QSGW are much smaller than (unsystematic) LDA errors. These errors due to neglect of the electron-hole interactions are corrected by scaled QSGW.

References