

Abstract Submitted
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Band gaps and band offsets in the SiO₂/Si interface calculated by including the self-energy of electrons and holes LUIZ FERREIRA, Universidade de São Paulo, Brazil, LEONARDO FONSECA, MAURO RIBEIRO, JR., Center Wernher von Braun for Advanced Research, Brazil — Density Functional theory, as formulated by Kohn and Sham (Phys. Rev. **140**, A1133 (1965)), is insufficient when it comes to the calculation of one-particle excitations (electrons and holes). In this case, one has to include the self-energy of the particle (see for instance R. Gómez- Abal. et al Phys. Rev. Lett. **101**, 106404 (2008)). This self-energy is mostly the classical electrostatic self-energy of the particle charge density but has an important contribution from exchange and correlation. In a recent paper (L. G. Ferreira et al, Phys. Rev. B **78**, 125116 (2008)), it is shown that the self-energy can be calculated with the help of a “self-energy potential”, wholly derived from pure atomic calculations. The band gaps calculated with those self-energies are precise, in no way worse than the GW band gaps, and yet the calculation is very simple and fast. Next challenge we faced was the calculation of the band-offsets of the all important Si/SiO₂ system. Notice that the “self-energy potential” is centered between two covalent bonded atoms in the Si side and centered at the O in the SiO₂ side. Then the question is whether these self-energy potential perturbations create a wrong charge density at the interface. The answer is that both gaps and band offsets were calculated with outstanding quality.

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