Calculations of electronic defects and excitons in oxides

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An overview will be given of calculations of self-trapped holes and excitons in amorphous and crystalline silica using the DFT/PBE approximation [1-3]. Processes leading to network degredation and the formation of oxygen interstitials as well as surface desorption have been identified. But, it is clear that this level of approximation is too crude in particularly for quartz where delocalized electronic states are lower in energy than localized ones. The reason is the spurious self-interaction in the DFT/GGA approximations to the energy functional. An implementation of Perdew-Zunger self-interaction correction [4] will be described and recent results on test systems (molecules) [5] as well as vacancy on a TiO2 surface discussed [6]. This correction makes the functional orbital density dependent (ODD) and unitary invariance of the orbitals no longer applies, giving rise to some additional challenges in the implementation. While significant, qualitative as well as qu antitative improvements in the calculated results are found, problems remain and more work is needed to make optimal use of the functional form where orbital density dependence is included.

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