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Defects levels and band alignments at semiconductor-oxide interfaces through the use of hybrid functionals[1]

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The issue of aligning defect levels with respect to the band edges at semiconductor-oxide interfaces is addressed through the use of hybrid functionals. The fraction of exact exchange contained in these functionals is responsible for a systematic increase in the band gaps, but leaves the energy levels of atomically localized defect states largely unaffected provided they are aligned with respect to a common reference potential. Hence, the location of the defect levels can be decoupled from the band-gap renormalization problem, which transforms into the determination of band edge shifts. Furthermore, band-edge shifts as determined within a hybrid functional scheme are found to give an accurate description of band offsets for several semiconductor-oxide interfaces. The combination of these results gives a viable framework for positioning calculated defect levels within a band diagram, which is directly comparable to experiment. Our approach is illustrated through several applications. More practical issues will also be addressed, including the differences originating from the choice of hybrid functional and the treatment of the exchange singularity in plane-wave formulations.

[1]Work carried out in collaboration with A. Alkauskas, P. Broqvist, F. Devynck, and H.-P. Komsa.