Determination of Defect Levels through Advanced Electronic Structure Methods

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Defect-level calculations performed through the use of semi-local density functional approaches generally suffer from severe band-gap underestimations, which lead to ambiguous results when attempting to determine defect levels within the band gap. More advanced electronic-structure methods such as hybrid functional and many-body $GW$ perturbation methods can nowadays be considered leading to band gaps in better agreement with experiment. However, it is not clear whether these advanced methods give consistent descriptions of defect levels, neither it is clear to what extent calculated defect levels are reliable with respect to experiment. This presentation precisely focuses on these issues. We determine charge transition levels with both hybrid functionals and $GW$ for a selected set of defects. In particular, we discuss how to overcome specific computational difficulties inherent to the adopted schemes. We show that defect levels of atomically localized defects as calculated with different electronic structure methods are consistent, provided the defect levels are given with respect to the average electrostatic potential. However, the position of the band edges may differ considerably. As experimentally determined defect levels are given with respect to the band edges, this indetermination leads to the appearance of a “band-edge problem”. Finally, we attempt to discriminate between hybrid-functional and $GW$ schemes by comparing our results to experimentally determined defect levels.