Exchange-correlation functionals for the band structure of solids: from bulk systems to interfaces and surfaces

Abstract:

I will discuss the results of recent benchmark studies in which we evaluate the quality of exchange-correlation functionals and pseudopotentials for the determination of electronic band gaps of solids[1,2,3]. We compiled for this benchmark a dataset with information on the experimental structure
and band gaps of 475 non-magnetic semiconductors.

I will then consider two first-rate functionals for band structures, namely the screened hybrid functional HSE and the modified Becke-Johnson exchange-correlation potential, and I will propose how to modify them to calculate accurate band alignments and defect energy levels at interfaces [4,5].

Our new local functionals [4,5] yield results of comparable quality as GW at a significantly reduced cost. This is because we account properly for the position dependence of electronic screening, through a density estimator of the local dielectric function.

References:

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