Topical Talk

What is the $G^{\text{W}0}$ band gap of ZnO? — Martin Stankovski

- Gabriel Antonius
- David Waroquier
- Anna Miglio
- Hémati Dixit
- Patrick Rinke
- Hong Jing
- Matteo Gianottamis
- Xavier Gonzalez
- Michiel Coey
- Gian-Marco Rigamass

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Zinc oxide is known to be a challenging system for $G^{\text{W}0}$ calculations. Its theoretical description has been widely discussed recently, and authors do not agree on the value of the band gap one should obtain from the $G^{\text{W}0}$ method. In an attempt to clarify the situation, we study the accuracy and the convergence properties of many schemes or approximations used at each level of the calculation, and show how different procedures may lead to very different conclusions. We first invest the sensitivity of the final band gap on the initial exchange-correlation potential used to generate the Kohn-Sham structure. We then study the behaviour of various plasmon pole models used to reproduce the dynamical properties of the dielectric matrix and discuss their validity for this particular system. Finally, the pseudopotential approach is compared to the PAW formalism, equivalent to all-electrons calculation.

Global exploration of the energy landscape of solids on the ab initio level — Klaus Doll


In the first step of rational synthesis planning, one needs to identify targets, i.e., (meta)stable crystal structures [1]. Simulated annealing has been shown to be one possibility to explore the respective energy landscape [2]. Our approach consists of a global search for structure candidates based on (up to very recently) empirical potentials, and subsequently a high accuracy local optimization. In order to overcome the limitation of employing potentials, ab initio energies are now used in all the stages [3-7].

After LiF [4] and BN [5], GeF$_2$ has been studied as an example of a system with a large number of crystal structures [1]. In the next step of rational synthesis planning, we will identify new targets, i.e., (meta)stable crystal structures, and subsequently determine high quality structures of new materials.

The surprising accuracy of semilocal functionals within density functional theory (DFT): A study of systems involving point defects — Rampi Rampasad

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The use of screened nonlocal exchange functionals within hybrid DFT computations is becoming practical, providing improved electronic structure descriptions [1]. However, the appropriate amount of nonlocal exchange (α) and the extent of screening (ω) to be used are still being explored. Here, we will focus on two properties relevant for semiconductors: charge transition levels and defect formation energies. By making the α and ω variables, it will be shown that semilocal treatments of the exchange interaction for defects in Si and ZrO$_2$ yield charge transition levels that are quantitatively competitive with more involved nonlocal treatments, extending notions presented recently [2]. This implies that the difference in formation energies
of neutral and charged defects remains a constant, although the formation energy itself may vary with the type of treatment. We have identified correlations between defect formation energies and features of the electronic structure of the defect-free parent material, allowing for extrapolations of the formation energy to the "correct" values.