

## Challenges for first-principles based properties of defects in semiconductors and oxides

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## EDITORIAL

## Challenges for first-principles based properties of defects in semiconductors and oxides

First-principles methods based on density functional theory (DFT) have been the mainstay of theoretical studies of the properties of semiconductor and oxide materials. Despite the tremendous successes of the past few decades, significant challenges remain in adapting these methods for predictive simulations that are quantitatively useful in predicting device behavior. Recent advances in computational capabilities, and improved theoretical methods taking advantage of ever more powerful computer hardware, offer the possibility that computational modeling may finally fulfill the long-sought goal of truly predictive simulations for defect properties. The exciting prospect of using modelling as ‘virtual experiments’ to obtain quantitatively accurate predictions of semiconductor behavior seems tantalizingly close, but challenges still remain, which is evident in the many divergent approaches adopted for the modelling and simulation of various aspects of defect behavior.

This special issue consists of papers describing different approaches to the study of defects, and the challenges that remain from the perspective of leading scientists in the field. It includes contributions on the theoretical and computational issues of using density functional methods for defect calculations [Nieminen], treatments to account for finite computational cell effects in periodic defect supercell calculations using analytical constructions [Lany and Zunger], or cell-size extrapolation techniques [Castleton *et al*], or instead using embedded cluster calculations to model charge-trapping defects [Shluger *et al*]. This issue also includes a description of the computation of  $g$ -tensor and hyperfine splitting for defect centers [Valentin and Pacchione], computation of vibrational properties of impurities from dynamical DFT calculations [Estreicher *et al*], and the use of DFT supercell calculations to predict charge transition energy levels of intrinsic defects in GaAs [Schultz and von Lilienfeld]. One contribution discusses the challenges of translating the results at the microscale into the macroscopic response of the material in a multiscale approach [Makov *et al*], and the issue closes with a discussion of neglected gaps in the first-principles modelling of defects, important problems that are commonly overlooked and perhaps deserving greater attention [Stoneham].

All papers were peer-reviewed following the standard procedure established by the Editorial Board of *Modelling and Simulation in Materials Science and Engineering*.

**Peter A Schultz**, Sandia National Laboratories, USA

**Guest Editor**