

Realistic calculations of surface optical properties: The influence of defects, self-energy and excitonic effects

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Surface optical spectroscopy allows for the real-time monitoring of semiconductor growth even in challenging environments, such as at high vapor pressures or under liquids. However, its full potential can only be realized if it becomes possible to calculate surface optical spectra accurately and with true predictive power. Such calculations have been difficult, due to the large numerical expense involved and the need to include many-body corrections in a number of cases.

Based on a massively parallel, real-space multigrid implementation of DFT-LDA [1] we have calculated reflectance anisotropy spectra in the independent particle approximation for a wide range of group-IV materials and III-V compounds [2]. Large surface reconstructions that occur during material growth are considered and contributions to the optical anisotropy from both surface and bulk layers are identified. We find that transitions between surface states give rise to specific “fingerprint-like” spectral features, but there also appear signals that are induced by the influence of the anisotropic surface potential on the electronic bulk wave functions and, to a smaller extent, by surface induced stress and relaxation in bulk layers. In addition, we show that surface defects have to be taken into account in order to explain some experimental results.

Using a model dielectric function [3] we are able to include electronic self-energy effects in the GW approximation. These effects lead to pronounced changes of the peak positions and line shape, substantially improving the agreement with experiment. An efficient algorithm for solving the Bethe-Salpeter equation allows us to go beyond the one-particle picture. For the controversially discussed model case of Si(110):H [4], we show in detail how electron-hole interaction and local-field effects influence the calculated spectrum and lead to quantitative agreement with the measured data.

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