Abstract

In the present thesis, the variational EXX method (varEXX) [78, 79, 80] has been implemented into a pseudopotential plane-wave code (S/PHI/nX [81, 82]). So far this method has been applied only for localized systems. By integrating it into the plane-wave framework it has been made applicable to periodic systems for the first time. The conventional approach of EXX is computationally very demanding. Subsequently performed tests of the new method indicate that varEXX allows a tremendous performance speed up while only a fraction of the memory consumption is required compared to the conventional EXX formulation. The efficient formulation of varEXX allows for a wide range of new applications. As an example it has been investigated whether exact exchange potentials can be considered as approximate linear functionals of the electron density. This is of significant importance concerning the practical use of EXX pseudopotentials. For the first time, DFT calculations using exact exchange pseudopotentials could be performed for GaN and InN with the complete semi-core-shell of the cations (3rd shell for Ga, 4th shell for In) being treated explicitly in the valency. Thereafter the results have been compared with those of calculations considering only the semi-core 3d- and 4d-electrons in the valency, respectively. A second focus of the thesis is the development of a generation scheme for ab-initio tight-binding parameters [122]. The method employs the formalism of GeneralizedWannier- Functions introduced by Marzari und Vanderbilt [116] and allows for a calculation of the electronic structure (eigenenergies and eigenstates) of huge systems with several thousands of atoms within the accuracy of the atomistic scale. This can be used for a computation of the optical properties of quantum dots based on foregoing DFT-EXX calculations in order to guarantee a correct description of the bandgap. Within the scope of this work effective ab-initio parametrizations for the GaN and InN bulk system have been developed and carefully tested with regard to their ability to an accurate description of the bandstructure.