Summary

Computer simulations are becoming increasingly important for developing new materials. This process is largely triggered by advances in our physical and mathematical understanding of materials and the recent progress in computer architectures. An important contribution of computational physics to material research and design is the development of highly optimized methods to accurately model material properties. The description of many material properties requires a seamless consideration of various length and time scales. Therefore, a new family of scale-bridging algorithms (multi scale) and algorithms combining various physics disciplines (multi physics) is currently in the focus of method development. Due to the huge computational demand of such methods and the tremendous running costs of high performance computing facilities, increasing the performance of the applied algorithms is critical. Due to recent advances in computer technology the development/optimization of novel algorithms becomes increasingly challenging. It requires a thorough knowledge of physics and numerics as well as state-of-the-art computer science. The gap which opens between physics and computer science creates a new interdisciplinary research field.

The objective of this thesis was the development and implementation of a new physics meta-language which simplifies the development of algorithms in computational materials design (CMD) significantly. (i) State-of-the-art computer science techniques have been applied or developed in this work to provide language elements to express algebraic expressions efficiently on modern computer platforms. (ii) Quantum mechanical algorithms are crucial in CMD. The new meta-language supports the Dirac notation to implement such algorithms in the native language of physicists. (iii) The language is completed by elements to express equations of motions efficiently which is required for implementing structural algorithms such as molecular dynamics.

A major goal of this work was to combine an intuitive algebra/physics programming interface with high runtime performance. Therefore, a major challenge was to allow the compiler to "understand" the algebraic or even quantum mechanical context. Only with this knowledge the compiler can generate machine code which is (at least) as efficient as manually optimized code. This has been accomplished by deriving new techniques, such as fully automatic BLAS/LAPACK function mapping, algebra type mapping, and the application of sophisticated template techniques. Further details like memory management, efficiently exploiting the computer's level caches and arithmetic pipelines which had formerly to be addressed by physicists are in our approach entirely shifted to the compiler. With the new technique of *virtual templates* the compiler can now even detect the quantum mechanical context of Dirac elements. While Dirac projectors, scalar products with metrics, Dirac operators, and Dirac vectors look syntactically very similar, this technique allows the compiler to recognize these terms and generate the proper highly efficient function calls. With virtual templates an interface which is strongly reminiscent to quantum mechanical textbooks could be provided. Equations of motions can be intuitively expressed exploiting *transformation pipelines* which we developed in this work.

In order to demonstrate the power of the this approach the full-featured plane-wave framework S/PHI/nX has been developed based on the new meta-language. The S/PHI/nX source code is remarkably short and transparent which simplifies code maintenance and the introduction of new sophisticated algorithms. The intuitive interface allows for a drastic reduction of the workload when implementing new CMD algorithms. Various benchmarks which have been conducted in this study compare S/PHI/nX with other state-of-the-art plane-wave packages with respect to runtime performance and accuracy. The obtained results indicate that the highly abstract S/PHI/nX approach yields a very high optimization level.

Since the computation of thermodynamic properties from first-principles requires very high accuracy and is computationally very demanding, computing these properties for a wide range of technologically important semiconductors provided a perfect benchmark to demonstrate the efficiency of S/PHI/nX. Based on these calculations we verified the general trends of phonon spectra, the location and amplitudes of the thermal anomalies of these systems. We compared our LDA and PBE data with the experiment and confirmed LDA to be a reliable basis for computing these properties for the class of III-V semiconductors in the zincblende phase.

With this work the new simulation package S/PHI/nX will be introduced which has been already applied successfully to a broad spectrum of systems, ranging from bio-inspired materials to metallic surfaces. The modular approach allows for a simple extension of S/PHI/nX with novel methods in future versions.