order.

The main focus of this work are studies of correlated electron systems near a Mott metal-insulator transition. In particular, we will present the first controlled DMFT calculation of the complete phase diagram of the fully frustrated single-band Hubbard model with semi-elliptic density of states at half filling using the QMC method. We will also perform the first calculations of the associated optical conductivity which do not depend on the assumption of anisotropy or disorder; these will be based on the general theory of densities of states and transport properties in high dimensions which is also developed in this thesis. In addition to these pure model studies, we will present results specific to the doped transition metal oxide $La_{1\text{-}x}Sr_xTiO_3$ which are obtained using the hybrid LDA+DMFT technique. This new method employs ab initio density functional theory in the local density approximation (LDA) for defining a general multi-band Anderson-Hubbard model which is then treated within the DMFT.

Structure of this Thesis

In chapter 1, we introduce the general electronic Hamiltonian and its reduction to the Hubbard model. We characterize the DMFT and its relation with mean-field approximations to spin systems and present the DMFT mean-field equations as well as their solution using the auxiliary-field QMC method. Finally, we discuss the analytic continuation of imaginary-time Green functions to the real axis by the maximum entropy method (MEM).

In chapter 2, we study the relations between lattice types, frustration, and densities of states (DOS). On the basis of Monte Carlo computations of momentum sums, we also evaluate the convergence of the density of states to its infinite-dimensional limit. We present new insights on the fractal tree commonly referred to as Bethe lattice and on the impact of longer-range hopping for this model. We develop a new formalism that allows to construct models with hypercubic symmetry which reproduce an arbitrary target DOS in the limit of infinite dimensionality ($d = \infty$). Using this approach, we can for the first time define a regular and translationally invariant lattice with semi-elliptic DOS in $d = \infty$.

In the central chapter 3, we thoroughly explore the low-temperature properties of the fully frustrated Hubbard model with semi-elliptic DOS within the DMFT. We determine the boundaries of a coexistence region of metallic and insulating solutions with high accuracy, thereby resolving a controversy on the existence of a first-order transition within this model. In the course of these studies, we detect and correct deficiencies in previously used QMC schemes and develop an improved criterion for the detection of phase transitions. Going beyond previous work, we also develop a method for a reliable determination of the first-order transition line and perform various tests of the accuracy of the result. Finally, we compute local MEM spectra and suggest some methodological improvements to be used in future calculations.

Transport properties are discussed in chapter 4, where we carefully review the formalism and its range of applicability and develop new expressions for the optical f-sum rule which are valid in $d = \infty$. We show that the correct consideration of