The rapid progress in miniaturization of electronic devices inevitably brings the current technology closer to a certain natural limit, when the manipulation of individual molecules, atoms or spins will constitute the basis for processing and storing information. Regardless of how distant this perspective seems to be, comprehensive understanding of physics at the nanoscale will certainly be of vital importance. The theoretical studies of transport properties of nanoscale systems, such as molecules, quantum dots or nanowires, due to strong electron correlations, are very demanding and the methods used are very often based on a series of approximations. Consequently, there are relatively few results that can be considered as benchmarks, and which can be directly compared to experiments. The aim of this project is thus to provide very accurate results and new predictions for problems that have not been studied yet. One of such open problems is undoubtedly the accurate quantitative calculation of transport characteristics in non-equilibrium conditions and the determination of dynamics with exact treatment of correlations. Therefore, the main goal of this project is to develop and adapt advanced numerical methods based on renormalization group techniques to study transport properties of correlated nanoscale systems, with particular emphasis on non-equilibrium and dynamical phenomena.

The considered nanostructures exhibit a number of exciting phenomena, not observed in bulk systems, resulting from the quantum nature of carriers and electron correlations. At low temperatures, such systems may exhibit the Kondo effect, which manifests itself in a universal increase of the conductance through the system. When a molecule or quantum dot is coupled to more independent conduction channels, the system may exhibit exotic Kondo states and quantum critical behavior. Within this project we will in particular analyze the non-equilibrium transport characteristics of molecules, such as molecular magnets, and their artificial counterparts, which can exhibit the two-stage or underscreened Kondo effects. In addition, for molecular and quantum dot systems, we will investigate the non-equilibrium heat conductance and the Seebeck coefficient, as well as the spin Seebeck coefficient in the case of junctions with ferromagnetic contacts. The next goal of the project is to analyze the time-dependent transport and quantum quench dynamics of correlated nanostructures. In this context, we will determine the time-dependence of the local density of states, which will allow studying the formation and evolution of the Kondo resonance. In the first stage, we will consider the time-dependent transport for molecular junctions and then the analysis of transport dynamics will be extended to hybrid nanostructures with superconducting electrodes. This will shed new light on the time-dependence of interplay and competition between different types of correlations, including electron pairing, Andreev reflection and the Kondo screening. Last but not least, we will also analyze the time-dependent transport for complex nanoscale systems exhibiting exotic Kondo states, such the non-Fermi liquid two-channel Kondo state, and quantum critical phenomena.

The topics covered in this project belong to modern research trends of nanoscience, including quantum and molecular spintronics, nanoelectronics, and quantum caloritronics, which are undergoing intensive studies in many leading research laboratories in the world. This is not only due to the fact that by analyzing the properties of nano-objects one reveals beautiful physics of purely fundamental nature, but is also stimulated by application possibilities in information storage and processing technologies, quantum computing, and energy harvesting at the nanoscale. The implementation of novel quantum devices is, however, a formidable challenge due to their complexity and various nontrivial phenomena as well as strong correlations that need to be fully understood and controlled. The goal of this project is to develop advanced numerical methods and to apply them to study the transport properties of correlated nanostructures, such as molecules and their artificial counterparts attached to external electrodes. This will allow for generating benchmark results and predictions about the dynamics and nonequilibrium transport in nanostructures, which could be directly compared with the current and future experiments. It can be expected that the results obtained during the execution of this project will, on the one hand, provide new and beyond the state of the art knowledge and understanding of transport properties of nanostructures, and, on the other hand, will stimulate further experimental research and exploration of new phenomena.