DESCRIPTION FOR THE GENERAL PUBLIC (IN ENGLISH)

The importance of microelectronic devices in the modern world is undisputed, being mainly a consequence of technological success in their miniaturization as well as mass production. However, further reduction of the size of traditional semiconductor electronic components becomes problematic due to the fundamental limitations of the physical nature. Molecular electronics offers a promising alternative to the well-established semiconductor-based electronics, paving the way for a boost in device miniaturization. The increasing interest in employing organic molecules as basic electronic components, such as switches, diodes, memories or transistors, calls for a thorough investigation and deeper understanding of the processes occurring in molecular junctions. Consequently, molecular electronics has recently become a field of intensive interdisciplinary research, both theoretical and experimental. Nevertheless, a number of phenomena associated with electronic transport in organic molecular systems still lack a full understanding, thus requiring a comprehensive theoretical study. In this respect, development of adequate theoretical methods of describing these phenomena as reliably and accurately as possible is of key importance for a further progress in molecular electronics.

Experimental investigations of the electronic transport characteristics of molecular systems utilize STM-like techniques and are usually performed at room temperature conditions. Hence, in the course of every single measurement of the tunneling current, which is repeated thousands of times to establish the macroscopic performance, the junction geometry inevitably changes with time, in quite an uncontrolled manner, as a result of thermal vibrations of its components, which permamently modify interactomic bonds within the molecule (in terms of both their length and relative orientation) as well as its connection to metallic electrodes. Variation of any of the structural parameters influences the electronic properties of the junction, and consequently, affects its transmission characteristics. Therefore, the result of a single measurement is in fact an average over distinct (and essentially not known in detail) junction conformations, whereas the macroscopic transport properties are concluded only upon another averaging of the results of the whole series of such measurements. On the other hand, most common theoretical investigations of the electronic transport in molecular junctions, which employ advanced *ab-initio* methods of solid state physics and quantum chemistry, are based on simulating the transmission spectra for a fixed junction geometry, usually corresponding to its ground state configuration at zero temperature. Such a methodology does not allow to take into account the above-described temperature-induced variations of the transport properties of the considered junction. This clear mismatch between the simplified model assumptions and the actual experimental conditions is often the source (apart from inaccuracy inherent to the applied theoretical methods) of serious discrepancies between theoretical predictions of the junction performance and the experimental reports.

In light of the above, the aim of our project is to develop and implement a more reliable description of the transport properties of a molecular junction by taking into account its structural evolution due to temperature effects. The proposed approach combines three complementary techniques into a consistent and verifiable methodology. First, ab-initio molecular dynamics simulations will be performed, at different system temperatures, to follow, in relevant time scales, the thermal evolution of the junction structure. Advanced methods of mathematical statistics and data mining will be then employed to analyze all the atomic configurations of the junction occurred in the course of its evolution, so as to classify them into clusters of similar structural characteristics. Thereby, the time-consuming computations of non-equilibrium transport properties will be performed just for a relatively small set of junction configurations representative for distinct clusters. Eventually, such obtained transmission spectra will be appropriately averaged to establish the macroscopic performance of the considered junction at the given temperature, comparable with experimental results. Within the project, this novel approach will be applied to several exemplary junctions composed of commonly studied organic molecules, including alkanes and biphenyls (with appropriate atoms or functional groups linking the molecule with the electrodes), in order to verify its versatility as well as predictive power.

By offering an adequate theoretical description of molecular junctions under experimental conditions, we should yield results in a better agreement with experimental data as compared to other approaches. Moreover, identifying the structural parameters of the system most crucial for the observed transport properties will help design molecular junctions that are thermodynamically stable in relevant temperature ranges — in terms of both their structure and electronic transmission characteristics — which is important for their prospective device applications. Thus, the outcomes of our project will advance the knowledge of electronic transmission phenomena in molecular systems, but also contribute to the ongoing search for molecular components exhibiting desirable electronic transport properties.