Controlled Mechanical Manipulation of Molecules

Sprawozdania

Informacje na temat projektu

CM3

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Podsumowanie kontekstu i ogólnych celów projektu

Nanotechnology developed from a purely theoretical vision pioneered by R. Feynman into a large, scientifically and commercially active field. In the course of this development the meaning of the word nanotechnology broadened, now including essentially all activities involving structures smaller than 100 nm. However, the original idea proposed by Feynman was to manipulate and control matter at

small – ultimately atomic – length scales and thus to establish a miniaturized fabrication technology in analogy to the macroscopic world.
The development of the (low-temperature) scanning probe microscope, the (LT-)SPM, an instrument with the capability to image and controllably move atoms, and the iconic IBM logo `written' with single Xe atoms on a Ni surface can be seen as the beginning of the experimental realization of atomic-scale nanotechnology in the sense proposed by Feynman. Yet, three decades since these first ground-breaking experiments, the question whether the technological paradigm of manufacturing can be extrapolated down to the molecular limit is still open.
The aim of the CM3 project was to develop controlled mechanical manipulation of molecules (CM3) using an LT-SPM to manipulate large organic molecules in three dimensions with optimal control over position, orientation and shape. During the course of the project, we identified the lack of information about the configuration of the molecule during manipulation, i.e. its shape, orientation and position, as the main obstacle to CM3. To address this problem, we designed and implemented a strategy with three components, modelling, validation and search, central parts of which were published in Scheidt et al. J.Phys.Chem. C (2023). We explored several ways of modelling molecular manipulation, ranging from simple surrogate models with few degrees of freedom to atomistic machine learning models trained on density functional theory calculations. Importantly, all models were either based on experimental data or benchmarked against experimental data to ensure their applicability. The main results have been published in Knol et al. Sci. Adv. (2021) and Ruiz et al. Commun. Chem. (2023). Finally, machine learning methods were used to solve the inverse problem of configuration monitoring by search, essentially creating a method to observe molecular configurations in real time during manipulation.
A second major outcome of the project was the direct application of molecular manipulation. Here we laid the foundations for turning scanning quantum dot microscopy (SQDM), which requires the placement of a single molecule on the SPM tip via manipulation, into a widely applicable method for imaging electrostatic potentials. Again using a three-component strategy, we designed and deployed specific control hardware, developed the theoretical framework for SQDM, and demonstrated various applications for studying nanoscale structures in the context of atomic and molecular manipulation. Our work paves the way for CM3 to become a game-changing technique for the study of molecular properties and molecular-scale engineering, combining for the first time fully deterministic manipulation with broad access to molecular degrees of freedom.

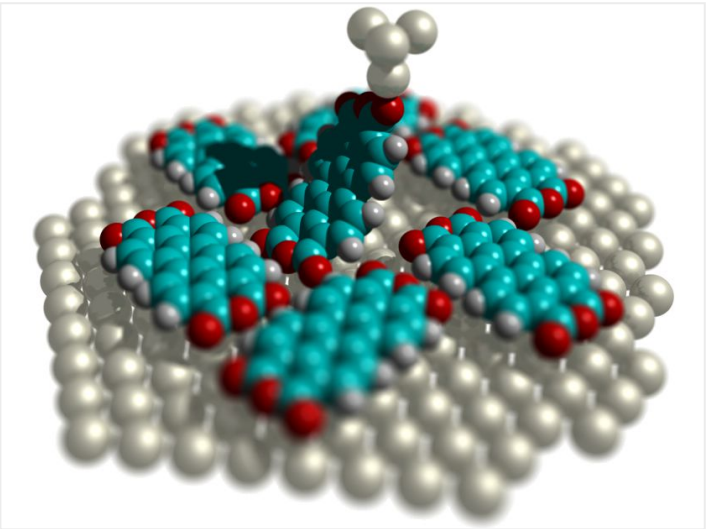
Prace wykonane od początku projektu do końca okresu sprawozdawczego oraz najważniejsze dotychczasowe rezultaty

CM3 is a project with a distinct interdisciplinary scope, uniting experts in several fields dedicated to solve a common problem. In the field of computational physics we have investigated the properties of individual molecules attached to metal bodies like surfaces or SPM tips in a variety of metastable conformations. The theoretical understanding gained by these calculations will allow us to make informed design choices when planning supramolecular structures and devices. We were also able to demonstrate the use of a first single-molecule device obtained from molecular manipulation: The sensor for a new microscopy type (scanning quantum dot microscopy) which is capable of revealing the weak electric fields around atomic-sized nanostructures. Finally, we were able to create and use a

machine learning agent, a computer program that could autonomously solve manipulation tasks by the principle of trial and error. Several individual steps in the field of computer science and machine learning have been made to solve the central problem of SPM-based manufacturing: The problem of observability. So far, the observation of molecular conformations during robotic manipulation remains elusive due to the dual role of the SPM tip as an actuator and an imaging probe.

Innowacyjność oraz oczekiwany potencjalny wpływ (w tym dotychczasowe znaczenie społeczno-gospodarcze i szersze implikacje społeczne projektu)

We have already implemented an algorithmic framework to solve the problem of observability and tested its performance on simulated (“synthetic”) problems. The next step, which will be crucial for reaching some of the anticipated goals of CM3, will be the application of this framework to the actual manipulation experiment. For this purpose we will improve the theoretical simulations of the manipulation process to capture the strength of the acting forces more accurately. Since a measurement of these forces is what we will use to reveal the molecular conformations, a good correspondence between simulation and experiment is needed for a good performance of the “observer” algorithm. Once we have achieved a sufficiently accurate conformation identification, we will continue the CM3 project in two directions: On the one hand, we will use the knowledge about the ad-hoc molecular conformation during manipulation to construct more complex metastable molecular assemblies which could have, for example, the properties of a motor. On the other hand we will use the knowledge of molecular conformations to study the properties of individual molecules in great detail. Many molecular properties which are relevant for future molecular devices (for example in the fields of electronic components or even quantum computing) rely on these properties which, in turn, depend strongly on the molecular conformation. Exploring this conformation-property relation will be the second central aspect of the second half of the project.



Manipulation of a single PTCDA molecule by the tip of a scanning probe microscope

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