Doctoral researcher

Investigating the ultrafast dynamics of individual molecules with terahertz scanning tunneling microscopy

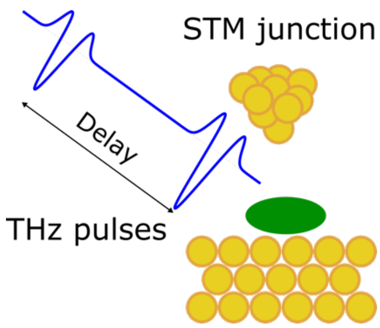
Contact:
Jun.-Prof. Dr. Manuel Gruber
manuel.gruber@uni-due.de
Tel.: +49203 37-92558
https://scholar.google.fr/citations?user=thqXVGwAAAAJ&hl=fr&oi=ao

Location:
Faculty of Physics
University of Duisburg-Essen
Lotharstraße 1-21
47057 Duisburg
Germany

Research project:
Functional molecules adsorbed on surfaces have attracted significant interest for their potential applications in memory storage and quantum computing. Our group mostly employs low-temperature scanning tunneling microscopy (STM) and X-ray absorption spectroscopy to control and investigate such systems. For instance, we manipulated the spin states of transition-metal complexes adsorbed on surfaces [1,2] and triggered molecular rotors [3] by injecting electrons of adequate energies. In addition, we investigated the many-body interactions of the molecule's magnetic moment with a metal [4] and a superconducting [5] substrate.

While the above studies allow a better understanding of physical and chemical phenomena taking place at the nanoscale, many questions remain open. For example, what exactly causes an electron to change the spin state of a molecule? The electron most likely excites vibrations, which eventually decay into a change in the molecule's conformation. A better understanding of the cascade of events leading to a spin-state change requires investigations at short time scales (sub-nanosecond).

To address these questions, we will use a pump-probe scheme where terahertz (THz) pulses are coupled to the STM junction to produce fast voltage pulses (~ 1 picosecond). The first pulse delivers electrons to trigger the dynamics under investigation, while the second pulse probes the state of the system after some delay. The time evolution of the microscopic processes (*e.g.*, spin-state switching) can be monitored by varying the delay between the two pulses. We have implemented and characterized such an instrument based on previous studies [6,7]. The main goal of the research project is to employ this instrumentation to probe the dynamics of selected molecules.



References:

[1] A. Köbke et al., *Reversible Coordination-Induced Spin-State Switching in Complexes on Metal Surfaces*, Nat. Nanotechnol. **15**, 18 (2020).

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[3] T. Jasper-Toennies, M. Gruber, S. Johannsen, T. Frederiksen, A. Garcia-Lekue, T. Jäkel, F. Roehricht, R. Herges, and R. Berndt, *Rotation of Ethoxy and Ethyl Moieties on a Molecular Platform on Au(111)*, ACS Nano **14**, 3907 (2020).

[4] M. Gruber, A. Weismann, and R. Berndt, *The Kondo Resonance Line Shape in Scanning Tunnelling Spectroscopy: Instrumental Aspects*, J. Phys.: Condens. Matter **30**, 424001 (2018).

[5] J. Homberg, A. Weismann, R. Berndt, and M. Gruber, *Inducing and Controlling Molecular Magnetism through Supramolecular Manipulation*, ACS Nano **14**, 17387 (2020).

[6] T. L. Cocker, V. Jelic, M. Gupta, S. J. Molesky, J. A. J. Burgess, G. D. L. Reyes, L. V. Titova, Y. Y. Tsui, M. R. Freeman, and F. A. Hegmann, *An Ultrafast Terahertz Scanning Tunnelling Microscope*, Nature Photon **7**, 620 (2013).

[7] T. L. Cocker, D. Peller, P. Yu, J. Repp, and R. Huber, *Tracking the Ultrafast Motion of a Single Molecule by Femtosecond Orbital Imaging*, Nature **539**, 263 (2016).

Profile of the candidate:

We are looking for a highly motivated candidate with a Master degree in physics or in a relevant field. The candidate is expected to have a good command of English and a solid background in nanosciences. Previous experience and knowledge in STM, ultrahigh vacuum, and pump-probe spectroscopy are highly appreciated.

Environment:

This project is part of the collaborative research center 1242 "Non-equilibrium dynamics of condensed matter in the time domain" (https://www.uni-due.de/sfb1242/). The selected candidate will integrate the integrated research training group of the CRC 1242 (https://www.uni-due.de/sfb1242/people_irtg.php), which offers a comprehensive training program in fundamental sciences and key soft skills.