Excited states and dynamics of molecular systems

T. Birk[1], L. Vogelsang[2], A. Bauer[1], F. Paschke[1], V. Enenkel[1], F. Liu[3], V. Romankov[4], J. Dreiser[4], A. A. Popov[3], R. Winter[2] and M. Fonin[1]

[1] *Department of Physics, University of Konstanz, D-78464 Konstanz*
[2] *Department of Chemistry, University of Konstanz, D-78464 Konstanz*
[3] *Leibniz Institute for Solid State and Materials Research, D-01069 Dresden*
[4] *Swiss Light Source, Paul Scherrer Institut, CH-5232 Villigen*

We report on the investigation of a molecular switch based on triazatruxene (TAT) molecule on the Ag(111) surface by means of scanning tunneling microscopy (STM) [1]. Inelastic electron tunneling (IET) excites a three-state switching with a particularly high degree of directionality of above 90% (**Fig. 1a,b**). The observation of directional switching upon IET excitation can be understood in the frame of Brownian ratchet model, assuming the excitation and diffusion within the periodic asymmetric potential landscape. We provide a detailed investigation of the impact of the measurement parameters and tip position as well as the role of the thermal noise on the switching and in particular on the observed directionality. We further investigate an arrangement of TAT molecules in a honeycomb structure which provides an opportunity to study the impact of fluctuating environment (simultaneously excited by the tunneling current) on the switching behavior of single TAT molecules. In the second part of the project, we focus on the single-molecule magnet $Dy_2@C_{80}(CH_2Ph)$ on graphene/Ir(111) and Au(111). STM measurements display ordered molecular islands after the electrospray deposition process (**Fig. 1c**). Using X-ray magnetic circular dichroism (XMCD) we investigate the magnetization dynamics of the molecular nanomagnets on a surface. We disentangle the continuous excitation related to the X-ray photon flux on the demagnetization dynamics and thus get the access to the main intrinsic mechanisms of magnetic relaxation in the system (**Fig. 1d**). Furthermore, we obtain a magnetic blocking temperature of $T_B(100) \approx 17$ K, which represents one of the highest values for surface-supported molecular magnets reported up to date [2].

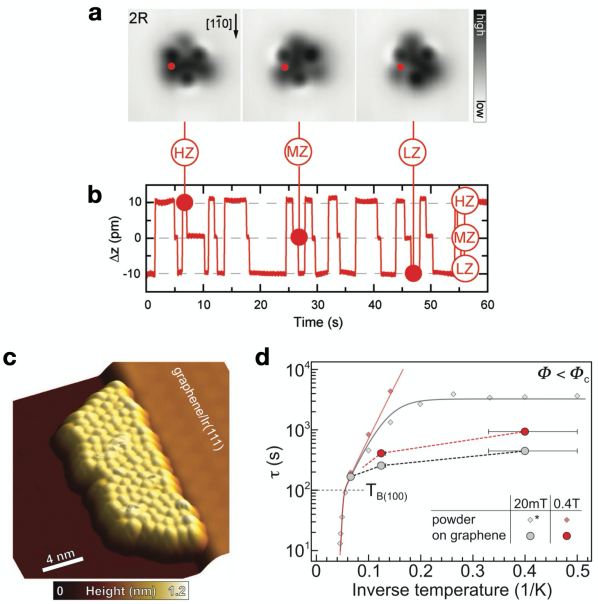

Fig. 1: ***(a)*** *STM images of the three states of the TAT molecule involved in the switching (10 mV; 100 pA).* ***(b)*** *Time dependence of the relative height of the tip recorded at 60 mV for the spatial positions marked in (a).* ***(c)*** *STM topography image showing an ordered $Dy_2@C_{80}(CH_2Ph)$ molecular island on graphene/Ir(111).* ***(d)*** *Temperature and magnetic-field dependency of the relaxation time as measured by XMCD. Diamonds and solid curves denote data obtained by SQUID on a bulk sample (data marked by asterisk is for 0 T) and corresponding fits, respectively.*

References:

[1] A. Bauer et al., *Adv. Mater* **32**, 1907390 (2020).
[2] F. Paschke et al., *Adv. Mater* **33**, 2102844 (2021).