

O 23: Poster Session - Electron-Driven Processes at Surfaces and Interfaces

Time: Monday 18:15–20:00

Location: P1A

O 23.1 Mon 18:15 P1A

Photoinduced carbon dioxide fixation by means of surface-functionalized silicon quantum dots with aromatic amines —

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In the last decade, the search for efficient methods able to capture, store and transform chemically atmospheric CO_2 has become a very dynamic research area. Several environmental issues such as global warming and climate change have been closely associated with the high atmospheric concentrations of this greenhouse gas. Here, a novel molecular system based on the use of surface-functionalized silicon quantum dots (sf-SiQDs) is theoretically explored as a proof of concept to bind CO_2 molecules. Within this scheme, CO_2 trapping is modulated by a photoinduced charge redistribution between the capping molecule and the silicon quantum dots (SiQDs). Chemical and electronic properties of the proposed sf-SiQDs have been studied with the Density Functional Theory (DFT) and Density Functional Tight-Binding (DFTB) approach along with a Time-Dependent model based on the DFTB (TD-DFTB) theoretical framework. Furthermore, a set of structural designs for capping molecules have been considered in order to strengthen the CO_2 binding energy. This study opens a new avenue to improve devices based on the use of sf-SiQDs for photochem-

ically activated CO_2 fixation.

O 23.2 Mon 18:15 P1A

Transmission of radio-frequency voltages to the tunneling junction of a scanning tunneling microscope —

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Electron spin resonance scanning tunneling microscopy (ESR-STM), as implemented by Baumann et al. [1], requires the application of a constant-amplitude radio frequency voltage at the tunnel junction over a wide range of frequencies (DC-40GHz). The constant amplitude is achieved by tuning the radio-frequency input power to compensate the variation of the transmission of the voltage line as a function of frequency [2]. However, this requires a precise determination of the radio-frequency transmission function. Here, we discuss the upgrade of a low-temperature STM with high-frequency cables and a superconducting magnet. The radio-frequency voltage applied to the tunneling junction has been measured for different frequencies to evaluate the transmission of the voltage line.

[1] S. Baumann, W. Paul, T. Choi, C. P. Lutz, A. Ardavan, A. J. Heinrich, *Science* 350, 417-420 (2015).

[2] W. Paul, S. Baumann, C. P. Lutz, A. J. Heinrich, *Rev. Sci. Instrum.* 87, 074703 (2016).