WORKSHOP #8
Wednesday, April 26, 2023
https://www.bnl.gov/usersmeeting/index.php

SPM User Meetup and Hands-on Open-source SPM Software "Hack a day" with Special Focus on Automatization of SPM

Organizers: Percy Zahl (BNL/CFN) and Thorsten Wagner (Johannes Kepler Universität)

This workshop aims to bring the SPM user community together to share latest science from HR-AFM to various SPM niche sciences. We discuss capabilities for remote or autonomous control of instruments and analysis of data.

The field of "Scanning Probe Microscopy (SPM)" is continuing to grow into diverse facets of scientific data acquisition. "Home built" or specialized microscope instruments require the control of various types of (nano) positioning mechanisms in combination with line by line imaging. In this meeting we would like to showcase capabilities of existing facilities, and particularly look forward towards new demands and opportunities in the field.
We plan on engaging participants to present their particular application and problems and provide an opportunity to meet the developers of existing facilities (in particular the developers of open source GXSM project *) in a dedicated "hack-a-day" like session — having virtually hands on microscope operation demonstrations.

Start Time (ET)	Title	Speaker (Affiliation)
8:00	Opening and introduction to task automatization with Gxsm	Percy Zahl, Thorsten Wagner* (BNL/CFN, * Johannes Kepler Universität, Linz, Austria)
8:30	Controlling the charge-state of individual molecules and promoting chemical reactions	Shadi P. Fatayer (Division of Physical Science and Engineering (PSE), King Abdullah University of Science and Technology (KAUST), Thuwal, Saudi Arabia)
9:00	Opening new routes of Scanning Thermal microscopy with Gxsm	Jean Spiece, Pascal Gehring (UCLouvain, Belgium)
9:30	Comprehensive single-molecular characterization of CoPc molecules on Ag (111) for surface catalysis applications	Xinzhe Wang (Yale University, CT)
10:00	Integration of GXSM with other instruments for automated data acquisition	Yoichi Miyahara / Noah Austin-Bingamon (Department of Physics, Material Science, Engineering and Commercialization Program (MSEC) Texas State University)

10:30	20 min Coffee Break / Chat Rooms	
10:50	Hack-a-day session ONE	Moderated by Percy Zahl and Thorsten Wagner
	Topics: *general Gxsm overview/updates,* *automatization, Python integration into GXSM, client/server options,* *various examples, Q&A*	
11:00		
12:30	1 Hour Lunch Break	
1:30	Characterization of Hydrogen Resist Lithography devices using Electrostatic Force Microscopy	José Bustamante (McGill University, Montreal, Canada)
2:00	Toward programmable electronic structures and molecular memories based on atomically precise graphene nanoribbons	Alexander Sinitskii, Mamun Sarker (University of Nebraska – Lincoln, Lincoln, NE)
2:30	½ Hour Coffee Break	
3:00	Hack-a-day session TWO	Moderated by Percy Zahl and Thorsten Wagner
	Topics: user demos/shares, Q&A	
4:00	15 min Break	
4:15	Closing remarks, outlook	Percy Zahl, Thorsten Wagner

ABSTRACTS (as available to date)

Comprehensive single-molecular characterization of CoPc molecules on Ag (111) for surface catalysis applications

Xinzhe Wang,[1] Percy Zahl,[2] Hailiang Wang,[3] Eric Altman,[1] and
Udo D. Schwarz[1,3]*
[1] Department of Mechanical Engineering and Materials Science, Yale University,
New Haven, CT 06511, USA.
[2] Brookhaven National Lab, Upton, NY 11973, USA.
[3] Department of Chemical and Environmental Engineering, Yale University,
New Haven, CT 06511, USA.

*Corresponding authors. E-mails: udo.schwarz@yale.edu

Abstract

Recently, Wang et al. [1,2] have found a promising class of hybrid catalysts based on Co-phthalocyanines (CoPcs) immobilized on carbon nanotube supports that promotes the production of methanol from CO_2. Thereby, the binding strength of the intermediate CO to the cobalt atom at the center of the CoPcs catalyst molecule has been recognized as a key descriptor affecting catalytic efficiency, with the ideal CO-Co binding strength being neither too strong nor too weak. To study this problem systematically at the single molecule level, we presented a comprehensive single-molecular characterization of CoPc molecules on Ag (111) using the custom-built low-temperature, ultrahigh vacuum scanning probe microscopy system. STM, AFM, 3D-AFM and KPFM techniques were carried out to characterize the CoPc molecule. We successfully identified the geometric structure, electron distribution, and barrier height distribution of a single CoPc molecule. The equilibrium distances and potential energies were also calculated across the molecule based on the 3D-AFM we preformed. A particularly noteworthy aspect of the approach is that after characterizing the molecule, systematically changing the substituents/side chains of the CoPc or the substrate the CoPc molecules sit on will allow to clarify the effect of these changes on the CO-Co binding strength and eventually allow us to fine tune the binding strength, which may open new avenues to optimize the catalytic reaction.

1. Wu, Y., et al., *Domino electroreduction of CO(2) to methanol on a molecular catalyst.* Nature, 2019. **575**(7784): p. 639-642.
2. Zhang, X., et al., *Highly selective and active CO(2) reduction electrocatalysts based on cobalt phthalocyanine/carbon nanotube hybrid structures.* Nat Commun, 2017. **8**: p. 14675.

Characterization of Hydrogen Resist Lithography devices using Electrostatic Force Microscopy

Jose Bustamante[1,3], Taylor Stock[2], Kieran Spruce[2], Yoichi Miyahara[4], Logan Fairgrieve-Park[1], Catherine Boisvert[1], Neil Curson[2], Peter Grutter[1]*

1 Physics Department, McGill University, 3600 rue University, Montreal, Quebec H3A 2T8, Canada

2 London Centre for Nanotechnology, University College London, London WC1H 0AH, U.K.

3 Departamento de Física, Universidad San Francisco de Quito, Quito 170901, Ecuador

4 Department of Physics, Texas State University, 601 University Drive, San Marcos, Texas 78666 USA

*Corresponding author contact: peter.grutter@mcgill.ca

Single dopant atoms in silicon are promising candidates for qubit hosts for the implementation of quantum computing. The plethora of techniques for fabrication of silicon semiconductor devices offers an attractive platform for the development of quantum technologies. Hydrogen Resist Lithography is a technique that enables the positioning of single dopant atoms of Phosphorus or Arsenic with atomic resolution on a silicon crystal [1]. This process can be used to fabricate quantum dots and electrodes over the surface of a silicon crystal with ultimate lateral resolution. Atomically defined Quantum Dots or single dopant atoms then arise as candidates for hosts of charge or spin qubits. So far, these devices have been characterized with transport measurements, and RF reflectometry [3]. However, Electrostatic Force Microscopy (EFM) offers an interesting alternative to characterize these devices using an AFM tip both as a probe to acquire topography and other material properties, and as an electric movable gate. EFM can also measure the energy levels of quantum dots and study the coupling between two quantum dots [2]. We have built an AFM capable of finding the relevant nanometer size structure in a macroscopic chip, imaging buried structures of dopant atoms, and detecting single electron tunneling events to QDs. I will present the instrument and discuss preliminary results in finding and characterizing hydrogen resist lithography devices.

[1] T. Stock *et al.* , ACS Nano **14,**3, 3316–3327 (2020).
[2] Y. Miyahara, A. Roy-Gobeil and P. Grutter, Nanotechnology **28**, 064001 (2017).
[3] X. Jehl, Y. Niquet and M. Sanquer, *J. Phys.: Condens. Matter* **28**, 10 (2016).