A Grant-in-Aid for Scientific Research on Innovative Areas
The Area Number 2509 (2013-2018)

MOLECULAR ARCHITECTONICS

MolArch

Orchestration of Single Molecules for Novel Functions

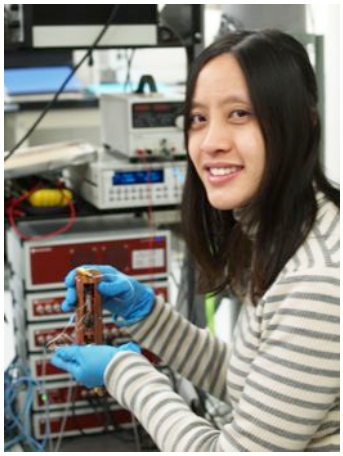
News Letter No.2 March 2014

Now at Work

A03 Prof. Tada's group

Thermoelectricity of molecular junction

We have been working on the thermopower measurement of molecular junctions because it gives fruitful information on the electronic structures of molecular junctions. Dr. Seekei Lee, who completed a doctoral program in Sep., 2013 and now working in Tada Lab as a project researcher, developed original scanning tunnel microscope (STM) to conduct the measurement. Her first project was to measure temperature dependence of electrical conductance of single molecular junctions when she joined the group in 2010. For this project, she decided to develop her original STM instead of using commercial one to gain ability to develop new techniques. The first machine was only capable of break-junction measurements; it had only z motion control. She improved her machine and succeeded in measuring effects of spin hybridization on the thermopower that was a main topic of her Ph.D thesis and will be published soon!



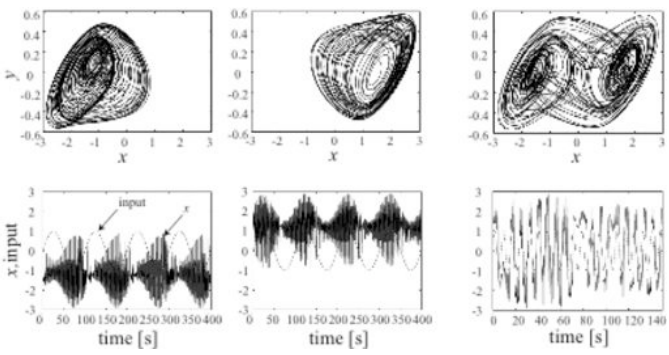
Dr. Lee holding her STM.

Achievement

A04 Prof. Tetsuya Asai

Chaotic resonance in forced Chua's oscillators

Stochastic resonance (SR) is a phenomenon in which dynamic noise is effectively used to induce state transitions in a double-well potential system driven by subthreshold input signals. The noises are supplied to the system as an additional force. Recently, a phenomenon called *chaotic resonance* (CR) has been spotlighted in the literature. CR can be observed in chaotic systems that have multiple strange attractors and the ability to accept subthreshold input signals; *i.e.*, such CR systems do not require any external noise source, unlike traditional SR systems. In this study, we employed Chua's oscillator as a candidate CR system. The oscillator was driven by a sinusoidal voltage source providing subthreshold input signals. In a certain range of input signal frequencies, we observed chaotic state transitions between the two attractors, whereas no state transition between the attractors was observed in the remaining frequency range. Furthermore, we observed nonmonotonic CR characteristics (correlation value and SNR between the input and the output signal) that corresponded to typical nonmonotonic SR curves.



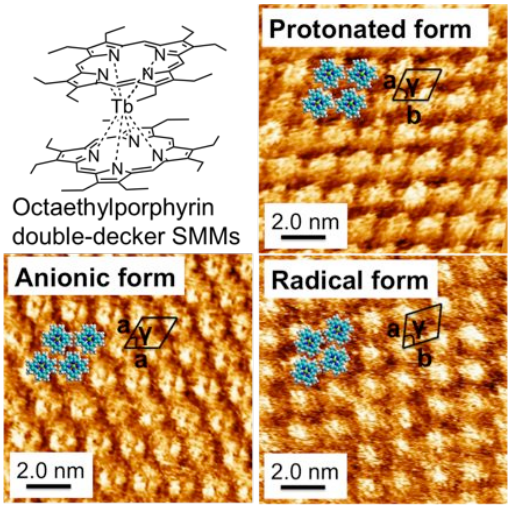
A01

Investigation of 2D supramolecular structure of porphyrin-based Tb(III) single molecular magnets

Ms. Tomoko Inose
(Osaka University)

During the last decade, phthalocyanine-Tb(III) double-decker single molecular magnets (SMMs) have attracted much attention because of their considerably higher blocking temperature.

In the present study, we focused on the porphyrin-Tb(III) double-decker complexes and their magnetic properties. In our previous study, we were successful in dramatically switching the magnetic property by synthesizing both the protonated and anionic forms of tetraphenylporphyrin-Tb(III) double-decker complexes. In this work, we tried to control the molecular alignment of SMMs on highly ordered pyrolytic graphite (HOPG) by self-assembly. We need to find the best 2D supramolecular structure of SMMs to realize future memory devices of SMMs. As a first step, we synthesized protonated, anionic, and radical forms octaethylporphyrin (OEP)-Tb(III) double-decker complexes and observed the molecular alignment on HOPG using scanning tunneling microscopy. In this study, we succeeded in isolating stable 2D structures of all OEP-Tb(III) double-decker complexes on HOPG.

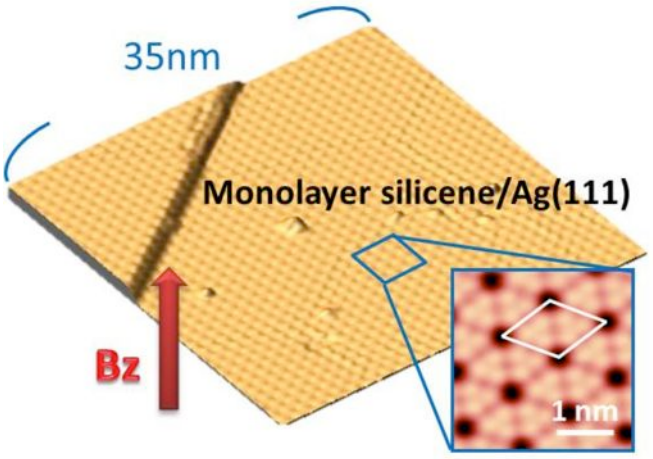


A02

Silicene- The new type 2D honeycomb structure consisting of Si

Dr. Chun-Liang Lin
(The University of Tokyo)

Silicene, the silicon version graphene has been successfully synthesized and also been regarded as a new allotrope of silicon structures. More than one phase of honeycomb structures were found on Ag(111) [1, 2], which indicating the bonding in silicene is much flexible than in graphene. Meanwhile the electronic properties were also studied. For single layer silicene as shown in the figure below, the serious symmetry breaking due to the interaction between silicene and substrate caused the absence of Dirac fermions [3]. Thus no Landau level was observed. For bilayer silicene, based on the interference patterns observer by dI/dV mapping, a parabolic band was found instead of a linear band [4]. Therefore the existence of Dirac fermion in silicene is still an open question. An approach to avoid undesirable effects from substrates is also prerequisite to realize the exotic properties of silicene.



1. C. L. Lin *et al.*, APEX **5**, 045802 (2012).
2. R. Arafune *et al.*, Surf. Sci. **608**, 297 (2013).
3. C. L. Lin *et al.*, PRL **110**, 076801 (2013).
4. R. Arafune *et al.*, PRL **110**, 229701 (2013).

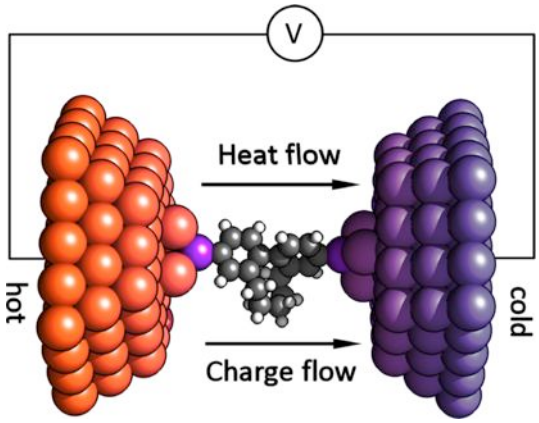
A03

Thermoelectric transport through single molecule junctions

Dr. Marius. E. Buerkle
(AIST)

The research field of utilizing single molecules in a bottom-up approach as building blocks of electronic devices is known as “molecular electronics”. It aims to further reduce size and energy consumption of present microelectronic circuits. Single molecule devices offer thereby a great possibility to tailor their properties by means of molecular design and chemical synthesis.

In our research, we aim to provide a theoretical description of the charge and energy transport mechanisms at the atomic scale, both from a fundamental and from a technological point of view. Recently we are focusing on thermoelectric devices based on single molecule junctions. For such systems it is necessary to describe not only the electronic but also the phononic degree accurately. Therefore we developed analogous to the electronic case a density functional theory based method to calculate the ballistic and non-linear phonon thermal conductance from first principles. With this extension of “molecular electronics” to “molecular phononics” we are now able to provide a comprehensive picture of the charge and energy transport in atomic scale devices.



A04

Sensing molecular charge dynamics by a GaAs-based nanowire FET

Mr. Shinya Inoue
(Hokkaido University)

Molecular materials should be key materials in future electronics and it is necessary to understand their electronic behaviors. However it is not easy task to characterize the charge dynamics of the molecular materials. My research subject is to develop the technique to detect the molecular charge dynamics using a semiconductor nanowire field-effect transistor (FET) (Fig. 1). The nanowire FET is very sensitive to the surface charges because of high surface-to-bulk ratio. We use a GaAs-based heterostructure for the FET channel, which has high charge-to-current conversion efficiency due to high electron mobility. We now investigate to detect the charge dynamics of Tetraphenylporphyrin (TPP). The TPP is drop-casted on the FET. By blue light illumination on the sample, the electrons excited in the TPP are stochastically exchanged between with the FET. We detect such dynamics in terms of the FET drain current noise. Measured noise spectrum shows a Lorentzian component together with conventional 1/f component (Fig. 2), which indicates the discrete charge event. Our next step is to detect such dynamics of the single molecule clearly by reducing the nanowire size.

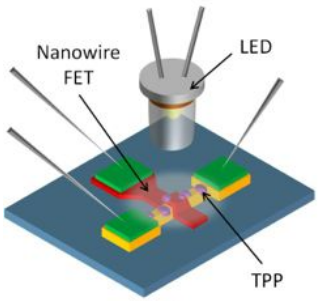


Fig.1

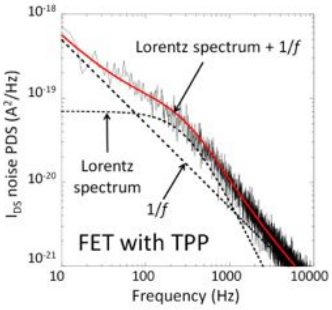


Fig.2

Report of the MolArch Meeting
11-12/Mar/2014, Sanjo Conference Hall, The University of Tokyo



The 4th meeting of Molecular Architectonics was held on March 11-12, 2014 at the Sanjo Conference Hall. 13 lectures and 47 posters were presented. There were more than 60 attendees, including members from our area and interested researchers.

Three speakers were invited from outside of our area. Prof. Hiroshi Nishihara (The University of Tokyo) suggested bottom-up strategies to construct nano-structures with the aid of step-wise synthesis. Prof. Manabu Kiguchi (Tokyo Institute of Technology) presented electronic transport properties of various metal-molecular contacts. Prof. Kazuyuki Aihara (The University of Tokyo) introduced novel numerical models for neural network and data processing in the brain. All these presentations were very useful toward advancing our research activities.

Prior to the meeting of Molecular Architectonics, out 2nd area meeting was also held on March 10, 2014 at the same place. First of all, we celebrated that the Japan Chemical Society (JCS) approved the Molecular Architectonics research community (president; Prof. Yoshihiro Asai (AIST)) as one of their official research associations. Additionally, each research representative presented their recent progress and their plans to collaborate on future studies.


Future Meetings

3rd Area Meeting
12-14, June 2014, Tendo, Yamagata

Edited by "Molecular Architectonics" Chief Office
1-3 Machikaneyama, Toyonaka, Osaka 560-8531
Mail: office@molarch.jp

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