



# MOLECULAR ARCHITECTONICS

Orchestration of Single Molecules for Novel Functions

*News Letter No.1*

November 2013

## Greeting from the representative



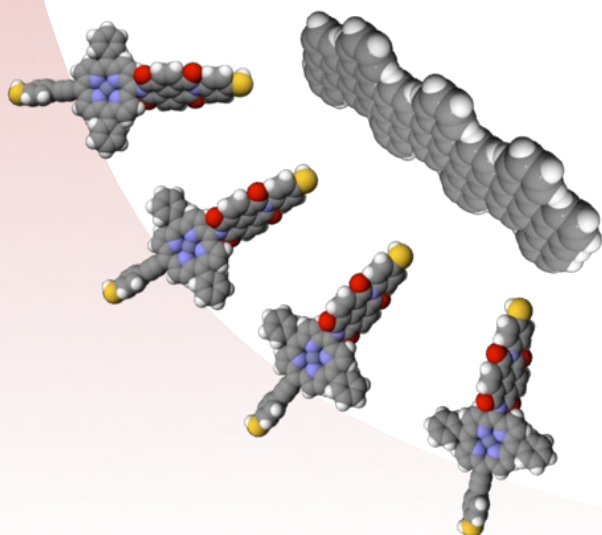
Prof. Hirokazu Tada  
(Osaka University)

A Grant-in-Aid for Scientific Research on Innovative Area, Molecular Architectonics: Orchestration of Single Molecules for Novel Functions kicked off. We are grateful to all those who gave us their cooperation.

The first stage of the research on measuring molecular conductance is characterized by spurious measurements for monomolecular films till 2000. During the second stage (till 2012), quantitative discussions became possible due to the establishment of the break-junction technique. Now we are in the third stage, where challenging efforts are made to achieve the desired functions by overcoming disadvantages of molecules, such as thermal instability and fluctuation.

For creating switching functions using light, electric and magnetic fields, a precise molecular design and a structural design of an electrode surface will be the foundation. We will realize signal processing by utilizing the fluctuations and variations in the current signals of molecules instead of randomly integrating single molecular devices.

Molecular architectonics refers to the manifestation of electronic, optical, and information-processing functions that are orchestrated by molecular assemblies like beams and columns in a building. The researchers will participate as “molecular architects”, participating in the design and fabrication of molecules to realize molecular functions by cooperative actions of numerous molecules. We hope the members enjoy research activities and put their best efforts into the challenging task of creating a new academic field.



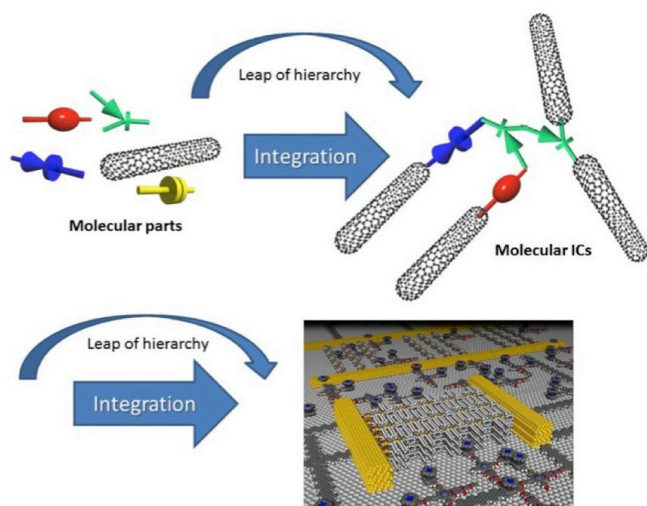
## ~Research Group Introduction from Leaders~



A01  
*Precise molecular design  
and synthesis*

Prof. Takuji Ogawa  
(Osaka University)

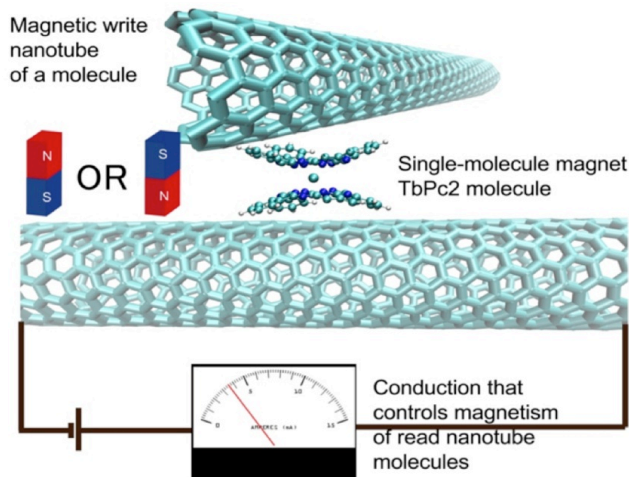
We design and synthesize functional organic compounds with the aim of realizing single-molecule electronics materials and integrated functional materials. The following are our specific targets. (1) We will perform molecular design and synthesis in order to use single molecules to realize functional units (such as rectification, negative differential resistance, memory, and integrated threshold device) that can be expected to express new functions through high-order integration. (2) We will develop anchor units for the metal electrodes and conductor units responsible for electrical conduction, and elucidating electronic states of charge transports and metal electrode-organic molecular interfaces. (3) We synthesize the stimulus-responsive molecules and use multi-probe measurement to identify the physical properties of the molecular assembly. We will also reduce these to single molecular elements and measure those electrical properties.



A02  
*Design and creation of  
surfaces and interface  
structures*

Prof. Tadahiro Komeda  
(Tohoku University)

We study the surfaces and interfaces that serve as the “stage” for molecular architectonics. Through the design, characterization, and control of the “foundation” of the “building,” we will establish basic structures for the two-dimensional molecular architecture. We will also examine the electronics state of molecular components fixed on the surfaces. Single molecules, magnetic molecules, stimulus-responsive molecules, and photo/electrochromic molecules will be synthesized by the A01 group, which possesses most advanced synthesis capability. Making the most out of access to unique molecules, we focus especially on establishing basic understanding as well as devising applications of intriguing phenomena generated by the spin/conduction electrons in a molecular unit. These results will be shared with groups A03 and A04, who will expand them to nano-gap devices. We also study theoretical models that will form the basis of a cooperative system, which is necessary for formulating the area of research.



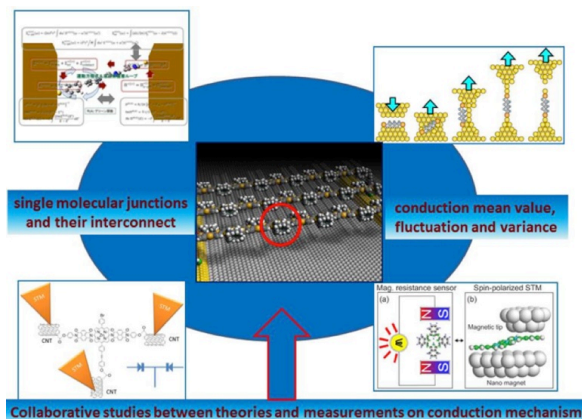




A03  
*Design and measurement  
of molecular function*

Prof. Yoshihiro Asai  
(AIST)

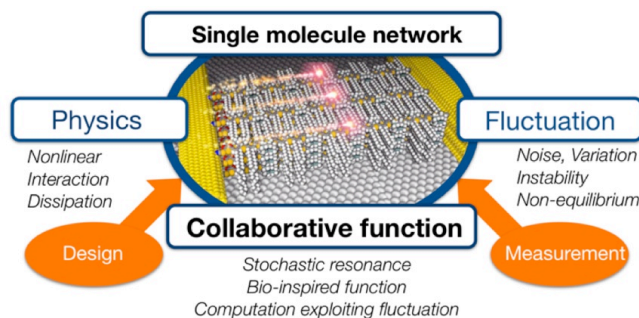
Fluctuation and variation effects on electric current and signal are common serious problems for all nanoelectronics devices. This problem hinders successful application of nanotechnology to electronics. In solid state devices, these are difficult to be characterized because of poor number of samples. Thanks to break junction methods which provide us thousands of experimental data in a very short time, there is the possibility in single molecular junctions. Our team will put our focuses on experimental and theoretical studies of mean transport values and their variations and/or fluctuations of single molecules and their small interconnects. Strong non-linear behavior in the current-voltage profile will be another focus. Well defined material science of fluctuations and variations which we are going to establish will provide us a rigid ground for nanoelectronics. In addition, interactions between single molecules through the substrate and/or the background of molecular framework architecture will be also investigated. By doing so, some functions of single molecular networks will be optimized based on the knowledge thus obtained from the bottom, i.e., at single molecular level. These studies will be done for electric and spin degrees of freedom, which will provide us wider extensions.



A04  
*Design and  
characterization of  
synergistic functions*

Prof. Seiya Kasai  
(Hokkaido University)

We design, implement, and characterize the cooperative functions in nonlinear element networks for molecular architectonics. The group will derive a new methodology and structural design guideline to exhibit cooperative functions for informatics exploiting fluctuations of molecules, rather than removing and suppressing them. Our basic strategy for such purpose is to utilize bio-inspired phenomena in nonlinear systems such as “stochastic resonance”, in which the response of the system is optimized or enhanced by noise, for example. We design single molecular networks, characterize the carrier transport and fluctuation in them, cause the stochastic resonance. We also design the nonlinear element network and characterize its responses. To find appropriate mechanism and establish technology for implementing information processing functions in the single molecular network, we extensively collaborate with groups A01, A02, and A03 in terms of molecular designing, synthesizing, and measurement. We integrate them with our knowledge and technologies of the nonlinear transport in nano-scale, stochastic resonance, nanodevice integrated circuit, and brain-inspired information processing architecture.

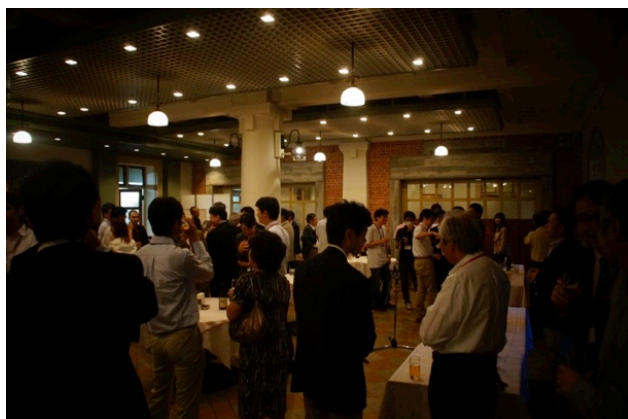


## Report of the Kickoff Meeting 30/Sep/2013, Osaka Central Public Hall



The kickoff meeting for the Grant-in-aid Scientific Research on Innovative Areas “Molecular Architectonics: Orchestration of Single Molecules for Novel Functions” was held on September 30, 2013 at the Osaka Central Public Hall. There were around 100 attendees, including members from out area and interested researchers.

The meeting was opened with a greeting from area representative, Prof. Hirokazu Tada (Osaka University). He gave an overview of the “Molecular Architectonics”. Then each leader of the four research groups talked about the research content and role of each group. The participants shared the concept and goal of molecular architectonics.



The concept of “Molecular Architectonics” was shared further through general discussion after the kickoff meeting. Prof. Shinji Murai (Nara Institute of Science and Technology), Prof. Hidetoshi Fukuyama (Tokyo University of Science) and Prof. Kazumi Matsushige (Shikoku University), who are evaluators of our area, gave us their congratulations and encouragement. The members of our area made up their minds to achieve the goal of molecular architectonics.

Many students from research groups in our area also attended the meeting and made the most of their time. We appreciate the cooperation from all the participants to make the kickoff meeting a success.



### *Future Meetings*

4th Molecular Architectonics Meeting  
10-13, March 2014, The University of Tokyo, open for all

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