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

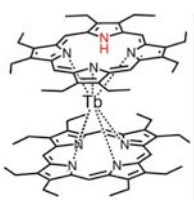
News Letter No.3 April 2014

Now at Work

A02 Prof. Komeda's group

Investigation of proton induced switching of the single molecule magnetic properties

The application of the freedom of spin and charge of an electron to the quantum process of information is called 'spintronics'. Single-molecule magnets (SMMs) are a unique class of compounds which show super-paramagnetic behavior at the "single-molecule scale". As molecular spintronics devices, they are attracted much attention because of controlling spin distribution and their unique energy barrier to magnetic relaxation. In the last two decades, many mono nuclear complexes showing slow magnetic relaxation have been reported. We investigate a Octaethyl-pyrrole (porphyrin) based Tb(III) double-decker complex which is stable with an unpaired π electron in their ligand's SOMO orbital as a radical form. Also theoretical research and NMR study indicate that if the proton exists on the one nitrogen of a pyrrole ring and the molecular coordination mode can be changed by protonation and deprotonation. It is possible to control their magnetic properties by controlling the spin distribution via molecule synthesis or the molecule adsorption-ordering in films such as with a redox reaction or pulse current application from a STM tip. This research is mainly conducted by Dr. Liu Jie.

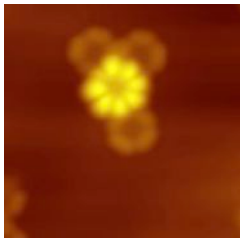


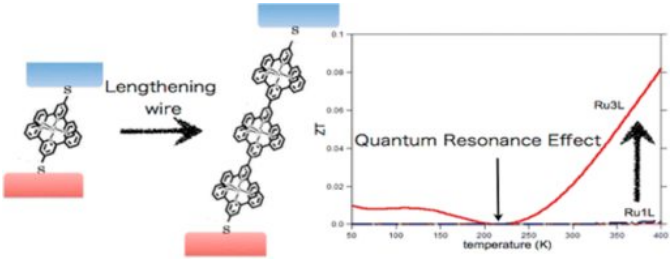
Photo : Dr. Jie and double-decker complex.

Achievement

A03 Dr. Hisao Nakamura

Thermoelectric Efficiency of organometallic complex

We presented a novel approach to obtain high thermoelectric figure of merit (ZT) for molecular junctions by quantum effect in the recent publication (H. Nakamura *et al.*, *J. Am. Chem. Soc.* 2013, 135, 16545). Superior long-range electric transport has been observed in several organometallic wires. Here, we discussed the role of the metal center in the electric transport and examinethe possibility of high ZT by controlling the quantum resonance effects. We examined a few metal center (and metal-free) terpyridine-based complexes by first-principles calculations and clarified the role of the metals in determining the transport properties. Quasi-resonant tunneling is mediated by organic compounds, and narrow overlapping resonance states are formed when *d*-electron metal centers are incorporated. Distinct length (L) and temperature (T) dependencies of thermopower from semiconductor materials or organic molecular junctions are presented in terms of atomistic calculations of ZT with and without considering the phonon thermal conductance. Higher ZT can be achieved by further designing of molecular orbitals and anchors.



A01

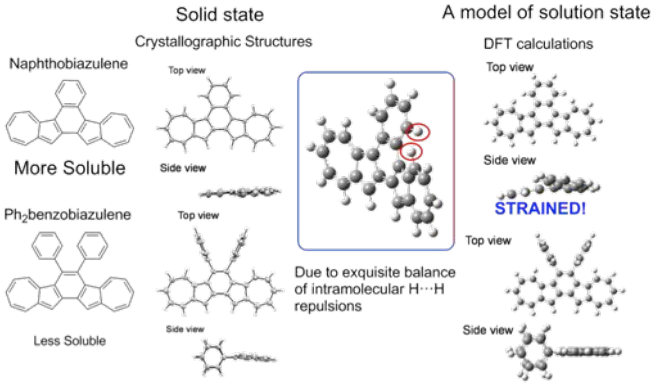
Synthesis of "cryptosoluble" polycyclic aromatic hydrocarbons

Dr. Takahiro Nakae
(Kyoto University)

Polycyclic aromatic hydrocarbons (PAHs) were promising functional optoelectronic molecules due to its rich pi-electron systems. We explore a novel function of PAHs by designing novel structures and syntheses.

Recently, we found that the newly synthesized naphthalene-fused biazulene molecule is more soluble than the benzo-fused one with rotatable phenyl groups. Naphthobiazulene took a planar structure in a solid state, however, assumed to be a bent structure in a solution state. We assumed that this phenomenon is controlled by the intramolecular H•••H repulsion. In a solid state, intermolecular packing force might overtake intramolecular repulsion, and took a metastable planar structure. In a solution state, naphthobiazulene could invert between bent conformers. On the contrary, benzobiazulene might keep a planar structure in the both states. We called solubility without any rotatable substituents as "cryptosolubility."

We are planning to synthesize functional cryptosoluble molecules and control their properties by external stimuli. We expected these functional molecules to play important role in the field of molecular architectonics.



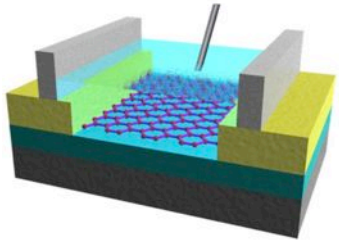
A02

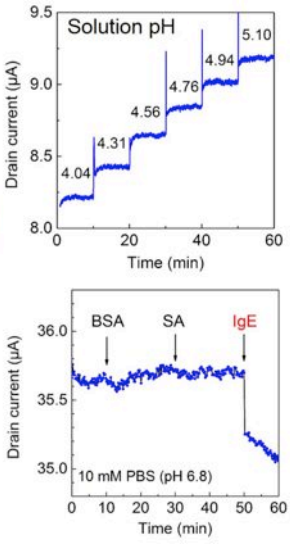
Graphene biosensors

Dr. Yasuhide Ohno
(Osaka University)

Graphene has very unique mechanical and electrical characteristics, such as high carrier mobility, chemically stableness and so on. Among many graphene based applications, it can be considered that biosensors are one of the most suitable applications because the sensitivity does not depend on the bandgap and its potential window is quite large. I have investigated that the graphene field-effect transistor (FET) based biosensors.

The drain current changed by solution pH change and protein adsorption, indicating that the graphene FET can detect charges in the solution. To realize the specific detection of biomolecule, various receptor modified graphene FETs have been fabricated. The aptamer-modified and fragment antigen-binding-modified graphene FETs showed specific protein detection. In addition, valinomycin (an ionophore for potassium ions)-modified graphene FET showed the specific ion sensing. These results showed graphene FETs have high potential for the practical applications.



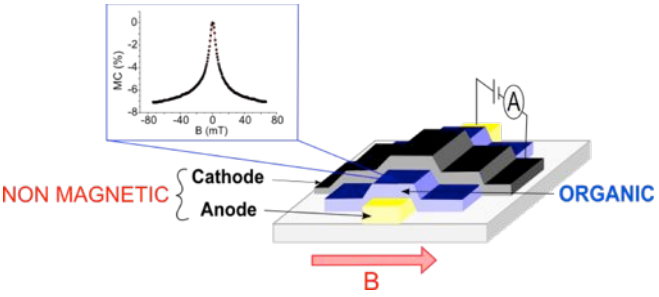


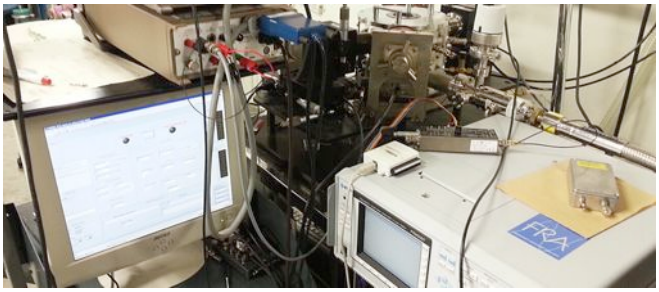
A03

Study of the magneto-resistance of organic semiconductors with impedance spectroscopy

Ms. Marine Fayolle
(Osaka University)

Organic semiconductors possess an interesting property: they show intrinsic magnetoresistance (aka organic magnetoresistance: OMAR) up to 20% at room temperature and low magnetic field (only a few mT) without ferromagnetic electrodes. The magnetoresistance can be switched from positive to negative just by changing the bias voltage, the thickness or the material, making it interesting for future application. This effect is explained by a several models involving various excited states such as bipolarons or excitons. In order to create application for OMAR, understanding the details of the mechanism is necessary. We suggest that impedance spectroscopy is the most suitable technique to study OMAR. By using this technique, we are able to gain insight into the behavior of the charge carriers in the semiconductor. A broad variety of information such as mobility of the carriers, the charge recombination processes, the role of traps in the device, as well as the processes at the interface can be investigated.





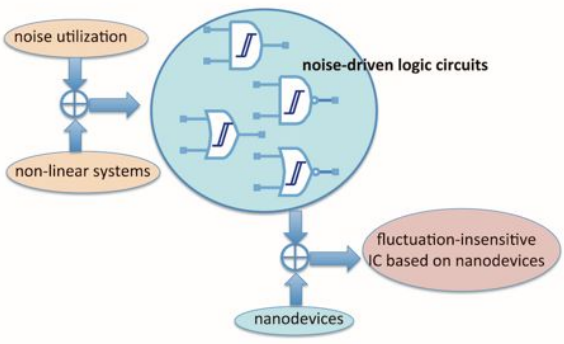
A04

Noize-driven logic circuit design for coarse-grain devices

Ms. Lizeth Gonzalez-Carabarin
(Hokkaido University)

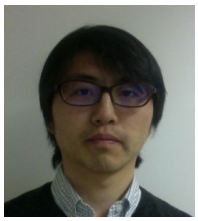
Current trends in electrical device miniaturization are lead by technologies such as nano-scale devices, whose aim is to take the device size to the limit of atomic or molecular scales. However, as such scales are reached, internal fluctuations are more evident in these devices that could affect the complete performance in terms of systems.

Our current work intends to overcome these problems by exploiting the benefits of noise in nonlinear systems to design fluctuation-insensitive digital circuits. Although our designs are based on MOS circuits, they are expected to be beyond MOS technologies, as a possible solution for overcoming fluctuations in nano-scale devices. Summarizing, our work offers three main advantages: one, the design of low power digital circuits, second, the design of fluctuation-insensitive circuits, and third, generation of a stable output, even if the circuit response depends on noise. It is also important to notice that synchronization becomes a major issue in digital synchronous design, since the time response depends on stochastic processes; therefore our current objective is the design of asynchronous circuits based on noise-driven digital circuits, since they allow delay-insensitive circuits.



New members joined!!

The following research representatives joined us from this April.





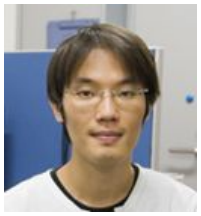
A01
Dr. Shohei Tashiro (The University of Tokyo)
Dr. Hiroshi Nishihara (The University of Tokyo)
Dr. Ken Albrecht (Tokyo Institute of Technology)
Dr. Michio Matsushita (Nagoya University)
Dr. Jun Terao (Kyoto University)





A02
Dr. Norihisa Kobayashi (Chiba University)
Dr. Yoshinori Yamanoi (The University of Tokyo)
Dr. Yasuo Yoshida (The University of Tokyo)
Dr. Toshihiro Kondo (Ochanomizu University)
Dr. Hiroshi Okuyama (Kyoto University)






A03
Dr. Akira Nakayama (Hokkaido University)
Dr. Manabu Kiguchi (Tokyo Institute of Technology)
Dr. Yoshiaki Sugimoto (Osaka University)
Dr. Yasuhisa Naito (AIST)




A04
Dr. Megumi Akai (Osaka University)
Dr. Hideo Kishida (Nagoya University)
Dr. Takeshi Yanagida (Osaka University)
Dr. Tsuyoshi Hasegawa (NIMS)

Future Meetings

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

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