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

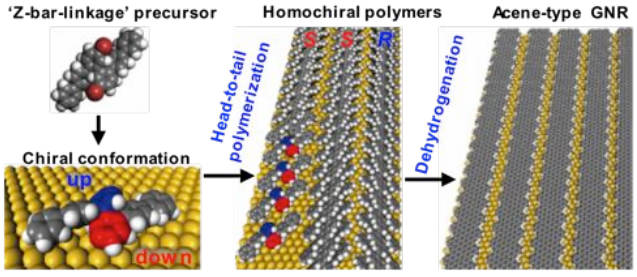
News Letter No.11 May 2017

Achievement

A03 Prof. Hiroshi Sakaguchi

Homochiral polymerization-driven selective growth of graphene nanoribbons

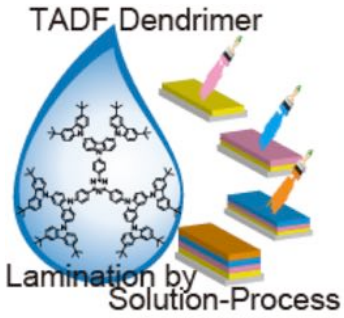
The surface-assisted bottom-up fabrication of graphene nanoribbons (GNRs) has attracted attention, due to ability to control the edges and widths of the GNRs precisely. The GNRs synthesis were consisted of the radical polymerization of precursors and following dehydrogenation, however the mechanism has remained unknown. Here, we demonstrate 'conformation-controlled surface catalysis': the two-zone chemical vapor deposition of a 'Z-bar-linkage' precursor results in the efficient formation of acene-type through optimized cascade reactions. These precursors exhibit flexibility that allows them to adopt chiral conformations with height asymmetry on a Au(111) surface, which enables the production of self-assembled homochiral polymers in a chain with a planar conformation, followed by dehydrogenation via a conformation-controlled mechanism. This is conceptually analogous to enzymatic catalysis and will be useful for the fabrication of new nanocarbon materials. (H. Sakaguchi *et al.*, *Nature Chemistry* 2017, 9, 57–63).

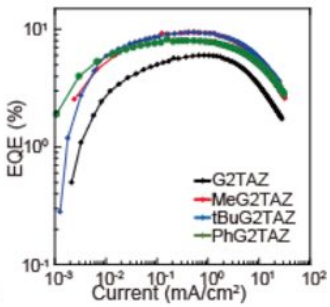


A01 Dr. Ken Albrecht
A03 Prof. Akira Nakayama

Solution processable thermally activated delayed fluorescence dendrimer

The development of emitting materials for OLEDs has started with fluorescence, moved to phosphorescence, and recently reached thermally activated delayed fluorescence (TADF). TADF has the advantage of a high internal quantum efficiency (up to 100%) and low cost (minor metal free). However, in our knowledge only one report of TADF material that can laminate other layers on top of it by solution process exists. We have developed new solution processable TADF dendrimers. OLED devices with the dendrimer and fully solution processed organic layers showed the maximum external quantum efficiency (EQE) of 9.5%. It is indicating that the dendrimer is harvesting the electrically-generated triplet excitons through TADF process. Thus, these dendrimers are TADF molecules for efficient OLEDs with fully solution processed organic layers. (K. Albrecht *et al.*, *Chemical Communications*. 2017, 53, 2439).



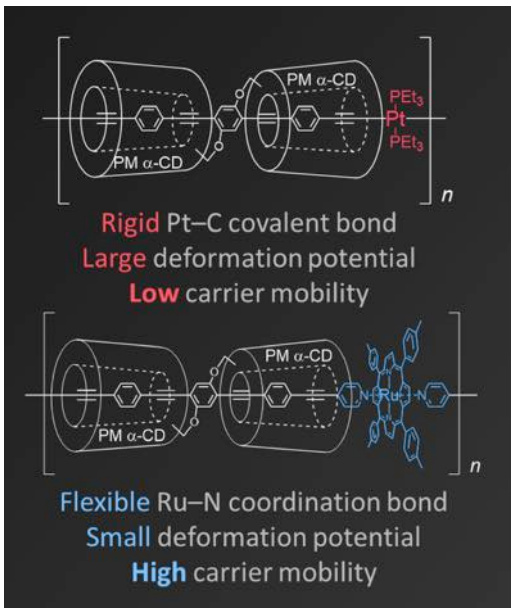


Achievement

A01 Prof. Jun Terao
A03 Prof. Hirokazu Tada

Carrier Mobility of Metal-containing Insulated Molecular Wires

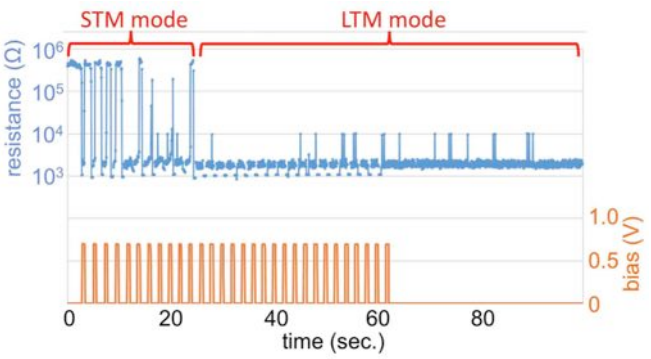
Organometallic molecular wire is a metal complex with π-conjugated polymers and the carrier mobility is an essential quality for wiring materials. The hole-mobility value of the all-carbon insulated poly(phenylene ethynylene) (PPE) wires decreased dramatically when organometallic units were introduced. However, ruthenium(II) porphyrin-containing insulated PPE wires exhibited a hole mobility comparable to that of the all-carbon PPE wires. We used first-principles calculations to investigate the hole mobility of metal-containing PPE insulated molecular wires. The metal–organic bond effects were considered using ruthenium(II) porphyrin–pyridyl and platinum(II) acetylide as the organometallic moieties. We found that high hole mobility can be achieved even when the metal–organic dπ–pπ interaction is weak. The weak metal–organic interaction reduces the structural deformation that accompanies hole hopping and compensates the reduced conjugation inside the molecular wire. Our results suggest a new principle for the design of functionalized metallopolymers with high carrier mobilities (T. Ohto et al., JPCC **120** 26637 (2016)).



A04 Prof. Tsuyoshi Hasegawa

Molecular-gap Atomic Switch

Gap-type atomic switch shows unique neuromorphic functions, such as a short-term memorization (STM) and a long-term memorization (LTM)-based learning. A vacuum gap of the switch enables a formation of a metal cluster on an electrode surface as well as a collapse of it, which is the origin of the unique function. However, the nanoscale vacuum gap is hard to fabricate in a high yield even using state-of-the-art fabrication techniques. In this study, we developed a new gap-type atomic switch using a molecular layer as a gap. We expect that a molecular layer also enables a formation and a collapse of a metal cluster on an electrode surface similar to the case of using a vacuum gap. The gap-type atomic switch using PTCDA molecule as a gap material shows a bipolar switching. It also shows STM and LTM-based learning, where the time constant is in the same order with those observed in operating a vacuum gap atomic switch (A Suzuki et al., in preparation). This successful result will be used in making an atomic switch network with the recent finding that p-type molecules also work as a gap-material (C. Lutz et al., JJAP, in press).

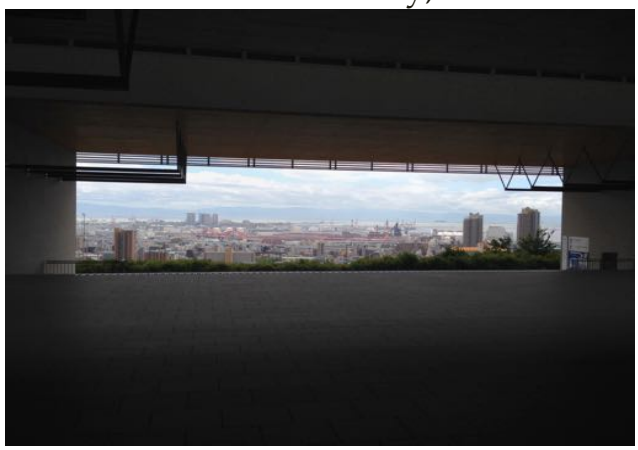


Joint Research Symposium of Three MEXT National Projects on Chemistry
18-19 November, 2016
Osaka University, Osaka

The Joint Research Symposium of Three MEXT National Projects on Chemistry was held on October 18-19, 2016 at Sigma-Hall, Toyonaka Campus, Osaka University, Osaka. All leaders of the three projects are professors of Osaka University. The symposium was aimed at reviewing the research topics of the three projects and broadening the research fields of all the members.

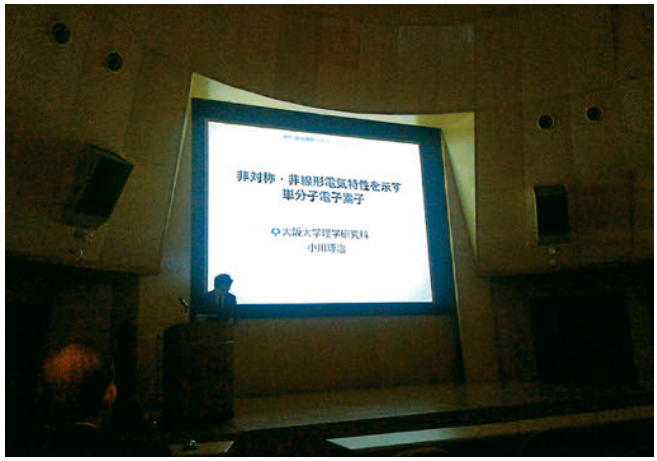
In this meeting, Prof. Hirokazu Tada firstly explained the aim of the symposium and then overviewed research work in the Molecular Architectonics area. From our area, Prof. Hirofumi Tanaka (Kyushu Institute of Technology), Prof. Yutaka Ie (Osaka University), and Prof. Ryo Yamada (Osaka University) gave talks about their research and collaboration in the Molecular Architectonics project.

10th Joint Research Meeting of MEXT National Projects on Condensed-Matter Science
9-10 December, 2016
Kobe University, Kobe



The 10th Joint Research Meeting on MEXT National Projects on Condensed-Matter Science was held on December 9-10, 2016 at Kobe University Centennial Hall, Rokkodai Campus, Kobe University, Kobe. The seven projects joining the meeting are as follows: Synergy of Fluctuation and Structure, Molecular Architectonics, Nano Spin Conversion Science, 3D Active Site Science, Topological Materials Science, J-Physics, and Synthesis of Mixed Anion Compounds toward Novel Functionalities. Researchers were also invited from six other projects.

From our area, Prof. Hirokazu Tada, Prof. Takuji Ogawa, and Prof. Ryo Yamada gave talks. They mainly spoke about the recent progress of design and measurement of molecular diodes and their rectification mechanisms.



6th Workshop for Young Researchers
16 March, 2017, Yokohama National University

The 6th Workshop for Young Researchers was held in Yokohama National University on March 16, 2017 and was well attended by approximately 15 students and staffs, despite the JSAP spring meeting and CSJ annual meeting being held at the same time.

This workshop was held to understand the each other's studies, and 12 researchers gave presentations of their recent research. Thanks to the members from Ogawa (A01) and Yamada (A03) groups, scanning tunneling microscope (STM) measurement became one of the hot topics in this workshop. STM measurement is one of the basic techniques for molecular electronics and important for attendees working with molecular electronics to know what research has been carried out.

Other topics were related to mechanically controllable break junction technique, molecular detection with semiconductor nanowire, and molecular devices. All attendees participated in active discussions in spite of the variety of the research topics.

These researches are essential for constructing "*molecular architectonics*". We hope that this workshop enhances the relationships between young researchers and to expands their knowledge.

Finally, we are grateful for the kind cooperation of the students of Prof. Oya group (A04) at Yokohama National University in holding this workshop.

(by Dr. Takashi Ikuta (A02))

Next Meeting

8th Area Meeting
2-4, June 2017, Osaka

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