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Satoshi Kaneko

# Design and Control of Highly Conductive Single-Molecule Junctions

A Focus on the Metal–Molecule Interface

Doctoral Thesis accepted by  
Tokyo Institute of Technology, Tokyo, Japan

 Springer

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# Supervisor's Foreword

A single-molecule junction, in which a single molecule bridges a gap between metal electrodes, has attracted wide attention due to its potential application in ultra small electronic devices and its unique structure. Despite these interests, there had been several issues for the investigation and practical application of the unique properties in the research field of the single-molecule junction studies. First, the conductivity of the single-molecule junction was very low. The reported conductance value of the single-molecule junction was smaller than the metal atomic junction by two orders of magnitude. Second, the atomic and electronic structures of the single-molecule junction under molecular conductance measurement were not clear. Most of single-molecule junction studies reported only molecular conductance. There were little structural characterization methods available for the single-molecule junctions and the structural details of the single-molecule junction were a black box. Third, there were little studies to show the novel functions or properties that were unique for the single-molecule junctions. The device performance of the single-molecule junction was generally worse than that of the bulk or isolated molecules.

Dr. Kaneko's thesis is on the high-performance single-molecule devices. He became a doctoral student of Tokyo Institute of Technology, Japan, in 2012 and joined the single-molecule junction experiment group. First, he has explored new generation of the metal–molecule interfaces formed by the direct  $\pi$ -binding. The interfaces made by the direct  $\pi$ -binding increased electronic conductance of the single-molecule junction up to the theoretical limit,  $1 G_0$  ( $2e^2/h$ ), which was the conductance of typical metal monoatomic contacts. Second, he developed a new characterization technique to see a single molecule confined between metal electrodes. This allowed us to reveal structural and electronic details in the single-molecule junctions. Based on the development in the metal–molecule interface structures and the spectroscopic characterization technique, he has searched for new functions of the single-molecule junctions. By governing the metal–molecule interface structures, the single-molecule switching function was realized.

His newly developed interface structure, newly designed characterization technique, and identification of novel function of the single-molecule junction will open the door for the future research field of the single-molecule devices.

Tokyo, Japan  
January 2017

Prof. Manabu Kiguchi

**Parts of this thesis have been published in the following journal articles:**

- Satoshi Kaneko, Tomoka Nakazumi, Manabu Kiguchi, “Fabrication of the well-defined single benzene molecule junction using Ag electrodes” *The Journal of Physical Chemistry Letters* **1**, 3520–3523 (2010), DOI: [10.1021/jz101506u](https://doi.org/10.1021/jz101506u). (chapter 4)
- Satoshi Kaneko, Lu Wang, Guangful Luo, Jing Lu, Shigeru Nagase, Satoru Sato, Michio Yamada, Zdenek Slanina, Takechi Akasaka, Manabu Kiguchi, “Electron transport through Single Endohedral Ce@C<sub>82</sub> metallofullerenes” *Physical Review B* **86**, 155406 (2012) DOI: [10.1103/PhysRevB.86.155406](https://doi.org/10.1103/PhysRevB.86.155406). (chapter 5)
- Satoshi Kaneko, Jinjiang Zhang, Jianwei Zhao, Manabu Kiguchi, “Electronic conductance of platinum atomic contact in a nitrogen atmosphere” *The Journal of Physical Chemistry C* **117**, 9903–9907 (2013), DOI: [10.1021/jp401562d](https://doi.org/10.1021/jp401562d). (chapter 6)
- Satoshi Kaneko, Yuuga Nakamura, Jingiang Zhang, Xiongbo Yang, Jianwei Zhao, Manabu Kiguchi, “Formation of single Cu atomic chain in nitrogen atmosphere” *The Journal of Physical Chemistry C* **119**, 862–866 (2015), DOI: [10.1021/jp510916h](https://doi.org/10.1021/jp510916h). (chapter 6)
- Satoshi Kaneko, Manabu Kiguchi, “Investigation on the pyrazine molecular junction studied by conductance measurement and near edge X-ray absorption fine structure” *Fullerenes, Nanotubes and Carbon Nanostructures* **22**, 166–172 (2014), DOI: [10.1080/1536383X.2013.798723](https://doi.org/10.1080/1536383X.2013.798723). (chapter 7)
- Satoshi Kaneko, Carlo Motta, Gian Paolo Brivio, Manabu Kiguchi, “Mechanically controllable bi-stable states in highly conductive single pyrazine molecular junction” *Nanotechnology* **24**, 315201 (2013), DOI: [10.1088/0957-4484/24/31/315201](https://doi.org/10.1088/0957-4484/24/31/315201). (chapter 7)

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