論文 / 著書情報
Article / Book Information

題目(和文)	単分子接合における化学反応
Title(English)	Chemical reaction on single molecular junctions
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出典(和文)	学位:博士(理学), 学位授与機関:東京工業大学, 報告番号:甲第10612号, 授与年月日:2017年9月20日, 学位の種別:課程博士, 審査員:木口 学,西野 智昭,河内 宣之,沖本 洋一,北島 昌史
Citation(English)	Degree:Doctor (Science), Conferring organization: Tokyo Institute of Technology, Report number:甲第10612号, Conferred date:2017/9/20, Degree Type:Course doctor, Examiner:,,,,
学位種別(和文)	博士論文
Category(English)	Doctoral Thesis
種別(和文)	論文要旨
Type(English)	Summary

（博士課程）
Doctoral Program

論 文 要 旨

THESIS SUMMARY

専攻： Department of	化学 専攻	申請学位（専攻分野）： Academic Degree Requested	博士 （ 化学 ） Doctor of
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要旨（英文 800 語程度）
Thesis Summary（approx.800 English Words ）

Since the molecular device has been proposed as a fancy dream in 1950s, the low dimensional world attracted many attentions over half of century. The molecular electronics, which contains a molecule (atom) as electronic component, which is different from the bulk. Within the nano-sized world, the new properties can generate. Thus, in the current work we take advantage of metallic nano junction explored the novel photochemical reactions.

In this thesis, the chemical reaction on metal atomic contact was focused utilizing the nano junction structure. All the experiments measured by mechanically controllable break junction (MCBJ) technique under the ultra-high vacuum (UHV) condition at 10K.

At the beginning, we constructed the available systems to investigate the chemical reaction on the metal atomic contact electron transport properties and the structural characteristics of the molecules relevant to the. First, we evaluated the Cu/H_2O contacts in experimentally and theoretically. The 0.1 G_0 peak was simulated by the calculation demonstrate the water presence could enhance the Cu atomic configuration with a wire. This special structure exhibited as a specific conductance peaks in the conductance histogram.

Moreover, we investigated systematically the electron transport properties of H_2O molecule with Au, Ag, Cu and Pt, totally for 4 metallic electrodes. All the metals we chose are able to work in a principle of surface plasmon. The conductance behavior indicated the formation of single water molecule junctions for the water–Au, Cu and Pt junction systems. The reaction strength were evaluated relied on the conductance histograms and plateau length histogram, in order of Pt>Cu>Au>Ag. With strong interplay of Pt, Cu with water attributed to obvious changes in the conductance behavior, on the other hand, the atomic chain offer more adsorption site of Pt enhanced the interaction strength. In contrast, absences of the atomic wire conformation lead Cu a well-defined peak in the conductance histogram. Oppositely, for the weak interactions between Au, Ag and water cases, the atomic chain leads the electrical transport properties in the nano junctions. Au atomic wire provides plenty of adsorption sites, achieve a slight change in the conductance behavior while without wire formation, Ag did not vary at all.

Also, the products, H_2, O_2/metal contacts has been considered. Here, we choose the Au, Ag and Cu for concern about further application. With comprehensively investigate the conductance histogram, length histogram, inelastic electron tunneling spectrum (IETS), we confirmed the H_2 and O_2 bridge in the metallic contacts. Additionally, *I-V* characteristics reveal Cu/H_2 with ratification behavior. For the hydrogen, oxygen/ metal contacts, the Cu electrodes performed discernable. The Cu/H_2 possesses a peak located around 0.3 G_0, besides, Cu/O_2 peak was observed at 0.1 G_0. Additionally, the vibration modes in the junction measured by the IETS also show potential for reveal the reality happened in the nano junction. Until here, we established of the identifications system of the water resolving reaction via conductance histogram and IETS. The further experiments would concentrate on the Cu/H_2O contacts.

Finally, rely on all the efforts we have done before, we explored the photochemical reaction, particularly, water photo-driven reaction in the Cu contacts excited by *UV-vis* light. The conductance histogram gave the evidence confirmed that electron transport properties of the Cu/H_2O contact changed with the irradiation. An additional peak was observed around 0.2 G_0 after excited by the *UV-vis* light. Vibration energies were investigated by IETS. The *dI/dV* curves and its differential spectra revealed that the ±40 meV with conductance located around 0.2 G_0 at zero bias corresponding to Cu-H_2-Cu configuration. Moreover, the conductance and vibration energy vary continuously as the function of excitation time has been considered simulate. The results demonstrate the H_2 derived from the reaction with the *in-situ* measurements. With the wavelength dependence investigation of the Cu/H_2O photocatalyst system, the results demonstrated the photoexcited produce at 400 nm drove by the $Cu_\chi O$ with Cu acting as co-catalysts, and the reaction excited under 600-700 nm illumination rely on Cu_n plasmon resonance.

As a summary, in this thesis, water decomposition reaction has been generated employed Cu nano electrodes. This finding demonstrated a high possibility of the single molecular junction becoming a powerful alternative solution of the current photocatalyst for water decomposition reaction. Additionally, the economical and easy-to-fabrication plasmonic materials, like Cu we used in this thesis can be considered.

Besides, *in-situ* reaction monitoring method relied on the conductance and vibration energies has been put forward. With this method, the experimental evidences for the reactions dynamics in the nano contacts can be evaluated at molecular junction. The molecular level understanding is foundation of precise-manufacture for the nano-sized devices, is the first step for application. Therefore, this method would make contributions to the molecular devices in the near future.

備考 ： 論文要旨は、和文 2000 字と英文 300 語を 1 部ずつ提出するか、もしくは英文 800 語を 1 部提出してください。