Usage Report for Fiscal Year 2020

Project Title:

Theoretical study of interaction between tunneling electrons and individual molecules at surfaces.

Name:
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1. Background and purpose of the project, relationship of the project with other projects

During the past decade, computer simulations based on a quantum mechanics have developed an increasingly important impact on solid-state physics and chemistry and on materials science. In field of material science, the surface chemistry is fundamentally important in many areas, such as molecular electronics, heterogeneous catalyst, fuel cell, etc. The adsorption of molecules onto a surface is a necessary prerequisite to any surface mediated chemical process. Understanding the bonding nature between the molecule and the surface on the basis of the electronic structure is therefore one of the most important issues in this field. The computational methods like density functional theory (DFT) have played a prominent role to elucidate the interaction between the molecule and the surface. Combination of DFT calculation and the method based on quantum many-body theory also provides a powerful approach to describe magnetism and dynamics on the surface with a high accuracy and efficiency. In addition, the computational method can be useful to study the details of energy transport and conversion among photon and electrons mediated with adsorbate at solid surfaces in the nanoscale regime. From the theoretical investigation of the adsorbed molecule on surface in combination with scanning tunneling microscopy and spectroscopy (STM/STS) experiment, we could expect the following research goals; 1) the deep understanding of the chemical/physical properties of an adsorbate on the surface not only in ground state but also in excited state, 2) the fine control of the chemistry on the surface. The overall purpose of our theoretical work is closely related with research goal - describing the details of energy transport and conversion at solid surfaces and interfaces in the nanoscale regime - of our laboratory, Surface and Interface Science laboratory.

2. Specific usage status of the system and calculation method

We have been studying the molecular adsorption on the well-defined metal surface using computational method in combination with experimental method. In our studies, first-principles simulations have been carried out using the Vienna Ab-initio Simulation Package (VASP) code and Quantum Espresso code in the density functional level of theory. The pure DFT methods have been mostly used and the inner electrons are replaced by projector augmented wave pseudopotentials (PAW). The climbing image nudged elastic band method (CI-NEB) is used to determine the transition states that are confirmed by imaginary frequency modes. In most of cases, STM image simulations are performed using Tersoff-Hamann approach. The computational results are compared with the available experimental result obtained from STM in our group. For the gas phase molecules, the Gaussian09 and Gaussian16 programs with atomic-orbital basis set are also effectively utilized to obtain stable geometries and corresponding electronic structures.

We also have been studying the many-body phenomena in molecular adsorption system, in particular the Kondo effect. The characteristic electronic state resulting from the Kondo effect, so-called Kondo singlet state appears as a sharp peak structure (Kondo peak) at the Fermi level (EF) in STS. In order to simulate the Kondo peak, we build numerical renormalization group (NRG) code and the STS simulation code based on the Keldysh Green's function method.

Electron-transport and luminescence properties of systems, that consist of a single molecule, substrate and the STM tip, are also our main research target. DFT calculations and the first-principles Green's function methods based on the many-body perturbation theory (MBPT) are used to investigate the basic properties of components, i.e., the adsorption nature of molecules and dielectric properties of the substrate as well as the excited electronic states of molecules with a high accuracy and efficiency. Based on the obtained results, we construct an effective model and investigate electron dynamics in transport and luminescence processes using the Keldysh Green's function method.

3. Result

(1) Molecular adsorption on solid surface: From single molecule to molecular network, and their optical properties [Emiko Kazuma, Minhui Lee, Jaehoon Jung, Michael Trenary and Yousoo Kim, Angew. Chem. Int. Ed. 59 (2020) 7960]

The mechanism study of plasmon-induced dissociation of a single-molecule strongly chemisorbed on a metal surface, two O_2 species chemisorbed on Ag(110) with different orientations and electronic structures, is investigated using a scanning tunneling microscope (STM) combined with light irradiation. The experimental study concluded that O_2 dissociation by plasmon is induced by hot-carrier transfer mechanism, especially for hole injection. To reveal the deeper understanding of detailed mechanism, we conduct the density functional theory (DFT) calculations.

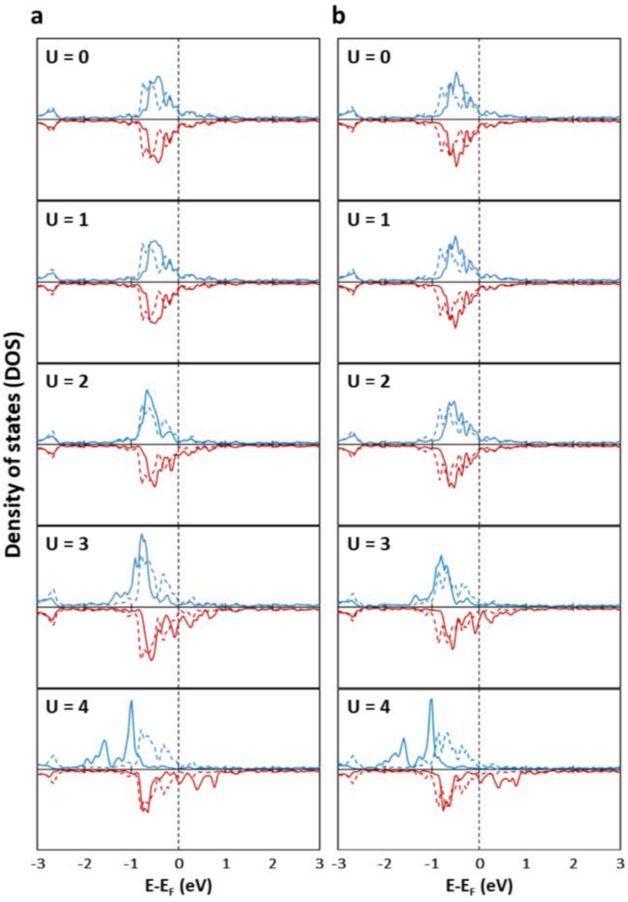

Figure 1. The calculated DOS of an $O_2[001]$ (solid lines) and $O_2[1\bar{1}0]$ molecule (dotted lines) on the Ag(110) surface with (a) DFT and (b) DFT-D3 calculations. The on-site Coulomb repulsion is applied to the oxygen 2p states with the DFT+U scheme (U = 0, 1, 2, 3 and 4 eV). Blue and red colors indicate the DOS of upper and lower spins, respectively.

The STM works show that the dissociation yield (Y_{STM}) was distinctly different depending on the sample bias polarity, the adsorbate states below E_F play a much larger role in the dissociation reaction than the states above E_F. This bias polarity dependence of the Y_{STM} can be interpreted based on the projected density of states (PDOS) on O_2 an Ag(110), which were calculated with DFT and DFT+U calculations. (Figure 1) The π^* states are distributed across E_F, and the DOS of the π^* states below E_F is much larger than that above E_F. In contrast, the bonding (π) states are distributed > 2eV below E_F regardless of the amount of effective Hubbard U parameter, U_{eff}. Therefore, charge injection to the π^* orbitals is the dominant excitation pathway in the dissociation of O_2 molecules on Ag(110) induced by the inelastic tunneling process with the STM. Furthermore, the much greater DOS of the π^* orbitals below E_F explains why hole injection is much more efficient at inducing dissociation than electron injection. The detailed reaction pathway is represented in Figure 2. Both hot carriers can simultaneously contribute to the dissociation but, the degree of contribution from hot-hole transfer and hot-electron transfer to the plasmon-induced chemical reaction is governed by the DOS distributions of the π^* states. When a hot-hole is transferred to the occupied π^* states of the O_2 molecule, its net charge becomes partially positive. The transient positive ion state formed by hot-hole transfer is dissipated to the vibrationally excited states according to a non-dissociative potential energy surface, and finally dissociation occurs.

A combination of quantitative analysis by STM and DFT calculation revealed that the hot carriers are transferred to the antibonding (π^*) orbitals of O_2 strongly hybridized with the metal states and that the dominant pathway and reaction yield are determined by the electronic structures formed by the molecule–metal chemical interaction.

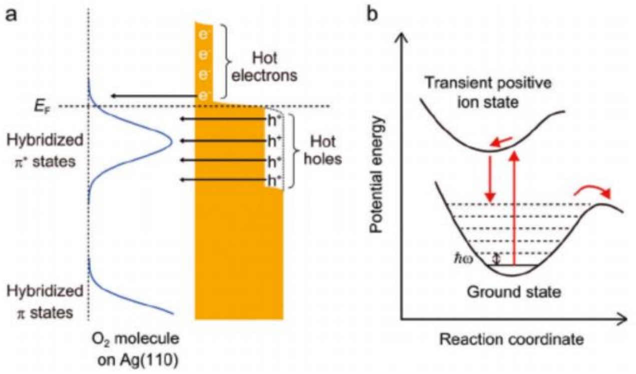

Figure 2. (a) Schematic model of the excitation mechanism for the plasmon-induced dissociation of a single O_2 molecules chemisorbed on the Ag(110) surface. Hot carriers (holes and electrons) are transferred to the strongly hybridized π^* states of the adsorbed O_2 molecules. (b) Illustrations of the potential energy surface for the plasmon-induced dissociation of the O_2 molecule induced by the hot-hole transfer to the occupied π^*states.

(2) Electronic structures of layered materials, such as graphene and dichalcogenide, and of framework materials, such as MOF and COF [Hyunseob Lim, Younghee Park, Minhui Lee, Jong-Guk Ahn, Bao-Wen Li, Da Luo, Jaehoon Jung, Rodney Ruoff and Yousoo Kim, Nano Lett. 20 (2020) 2107]

We verify the formation of $C_6(OH)_1$ and its electronic structure using periodic density functional theory calculations which is synthesized in experiment. The chemical route for formation of centimeter-scale stoichiometric "graphenol (C_6OH_1)", a 2D crystalline alcohol, is reported via vapor phase hydroxylation of epitaxial graphene on Cu(111). The higher-resolution STM image (Figure 1a) obtained by the molecule-modified tip visualizes the exact bonding site of the functional group and the proposed model structure of hydroxylated graphene, that is, graphenol, in the dotted rectangle of Figure 3a is shown in Figure 3b with a height profile along the orange-dotted line.

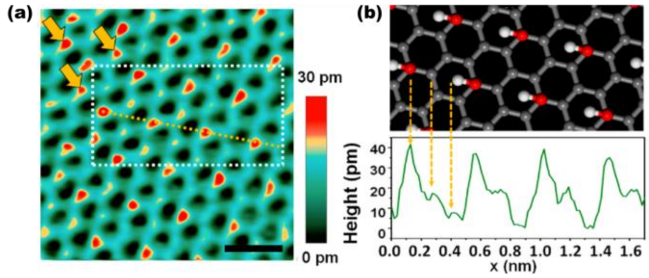

Figure 3. (a) High-resolution STM image of EG-OH surface by a molecule-modified STM tip. Scale bar, 0.4 nm. (b) The predicted atomic configuration and height profile along the yellow dashed line in panel a.

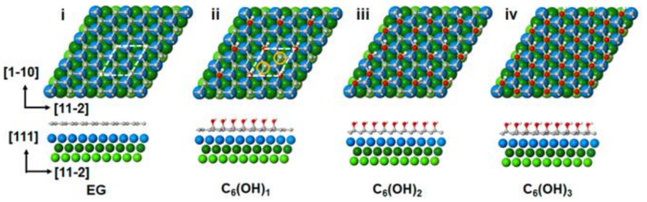

Figure 4. The optimized atomic geometries for EG, $C_6(OH)_1$, $C_6(OH)_2$, and $C_6(OH)_3$ [first, second, and third Cu layers: blue, dark green, and light green spheres, respectively]. The $(\sqrt{3} \times \sqrt{3})R30°$ unit cell employed in the periodic DFT calculations is denoted with a white parallelogram.

Periodic density functional theory (DFT) calculations were carried out to further understand the formation of $C_6(OH)_1$ and its electronic structure. The optimized geometries of epitaxial graphene (EG), $C_6(OH)_1$, and $C_6(OH)_2$ that were observed by STM are presented in Figure 4a-i to iii. Because the two carbon atoms at the meta positions (marked with yellow circles in Figure 4a-ii) with respect to the hydroxyl groups remain unbonded in the unit cell of $C_6(OH)_1$, we also studied the fully functionalized superstructure, that is, $C_6(OH)_3$, despite its absence in STM observations (Figure 4a-iv). The formation of a C-OH σ-bonding induces sp^3 character not only to the carbon atom bonding with −OH but also to its neighboring carbon atoms which may, therefore, interact more strongly with the Cu atoms beneath them. These C-Cu distances are 2.18, 2.07, and 2.01 Å for $C_6(OH)_1$, $C_6(OH)_2$, and $C_6(OH)_3$, respectively, which are significantly shorter than the interfacial C-Cu distance (3.18 Å) of EG/Cu(111) before functionalization (Figure 4). The computationally evaluated binding energies per one −OH group (E_b/OH) in the unit cell of EG/Cu(111) are −2.23, −2.19, and −1.98 eV for $C_6(OH)_1$, $C_6(OH)_2$, and $C_6(OH)_3$, respectively. Considering the sequential binding of an −OH group to EG, the calculated E_b of the second and third −OH are smaller than that of first −OH by 0.09 and 0.67 eV, respectively. The significant decrease in E_b for the third hydroxylation can, therefore, reasonably explain our not observing $C_6(OH)_3$.

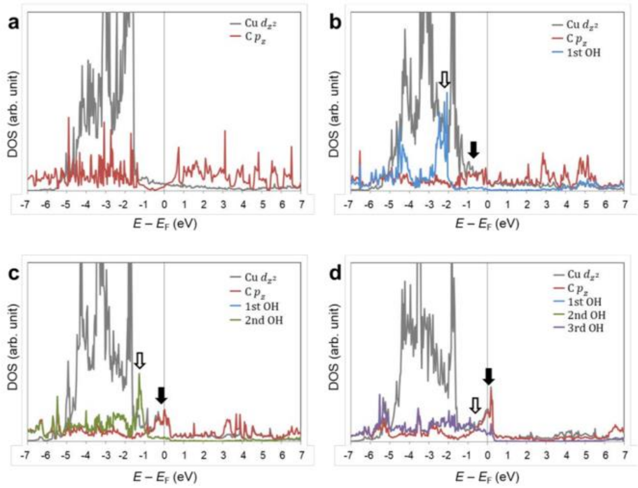

Figure 5. Projected density of states (PDOS) for the d_{z2} state of the Cu substrate and the p_z state of epitaxial graphene (EG), and the local density of states (LDOS) for the hydroxyl functional group on EG: (a) EG/Cu(111), (b) $C_6(OH)_1$, (c) $C_6(OH)_2$, and (d) $C_6(OH)_3$ superstructures.

The decrease of E_b for second and third hydroxylation is also represented in the electronic structure which is modified by functionalization with -OH groups (Figure 5). The prominent features of interfacial interaction between the Cu substrate and π states of EG, i.e., the Cu d_{z2}– C p_z interaction near the Fermi level (E_F) are indicated with filled arrows, and the LDOS positions near the E_F of the hydroxyl group binding to EG are indicated with unfilled arrows. Moreover, The characteristic features of the Dirac cone are significantly destroyed by further functionalization of EG/Cu(111), that is, $C_6(OH)_2$ and $C_6(OH)_3$ (Figure 6).

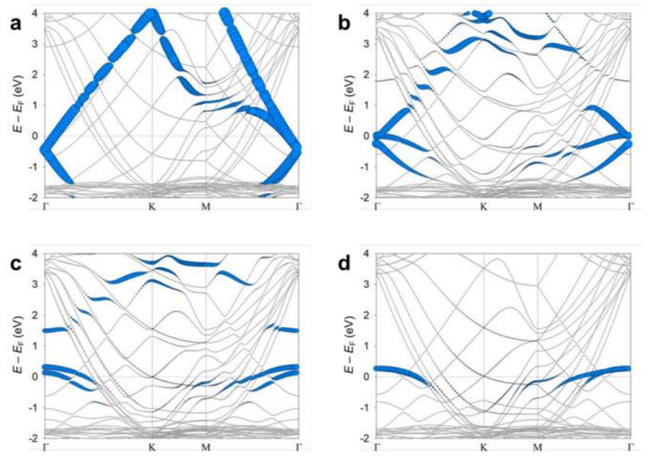

Figure 6. Band diagram for (a) epitaxial graphene on Cu(111), EG/Cu(111), (b) $C_6(OH)_1$, (c) $C_6(OH)_2$, and (d) $C_6(OH)_3$ superstructures. The relative amount of C $2p_z$ character is proportional to the size of the blue dots.

(3) Raman spectra of self-assembled monolayers on gold electrode

We are developing new experimental technique, tip-enhanced Raman spectroscopy (TERS) in liquid environment, to achieve nanoscale Raman signal mapping of organic molecules on metal electrodes with local structural properties. While a gold tip enhances the incident electric filed as much as 100, TERS measurements still reacquire the highly Raman active molecules to be studied because the long accumulation of the Raman signal is hampered by instrumental instability. It is thus prerequisite to systematically study the Raman intensity as well as the vibrational energy for the various kinds of organic molecules (self-assembled monolayers (SAMs) on gold electrode). In this study, we have succeeded in obtaining Raman spectra of benzyl mercaptan ($PhCH_2SH$) adsorbed on gold clusters (Fig. 7(a)). We found that the simple gold dimer model is enough to reproduce the experimental Raman spectrum (Fig. 7(b)).

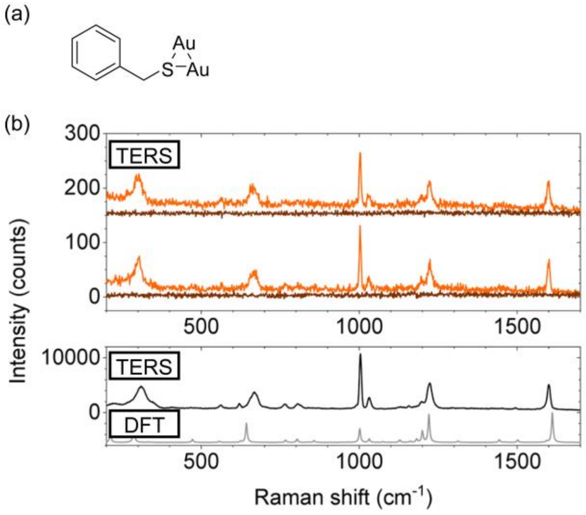

Figure 7. (a) Molecular cluster calculated in this study. (b) Experimental and calculated Raman spectra of $PhCH_2SH$ SAM.

(4) On-surface photo-induced reactions and syntheses

On-surface intermolecular coupling reaction of alkynes was systematically studied in FY2020. This molecular system is explored by the combination of STM/STS and DFT calculations. More importantly, the tip-enhanced Raman spectroscopy (TERS) technique has been successfully integrated into this study, and it was used to experimentally judge the core chemical groups involved in the reaction intermediates or products at the single-chemical-bond level based on the corresponding vibrational modes.

Highly unsaturated π-rich carbon skeletons are versatile in tuning the structural and optoelectronic properties of low-dimensional carbon nanostructures. However, precise chemical identification and controllable integration of the target sp-/sp^2-carbon skeletons during synthesis are challenging and elusive. In this study, the π-skeletons generated by the coupling of terminal alkynes were visualized and identified at the single chemical bond level both topographically and spectroscopically, and further bond control was demonstrated. By a combination of STM/STS and TERS techniques, we precisely revealed the generated sp-sp^2-carbon skeletons in real space as evidenced by their characteristic topographies and localized electronic and vibrational properties. Furthermore, by applying voltage pulses from the STM tip to the target molecules, bond control is achieved resulting in the dehydrogenative transition. DFT calculations further validate that the lowest unoccupied molecular orbital derived densities and the CC stretching modes of sp-carbon are valuable in recognition of π-skeletons. This study shows the versatility of spectroscopic information in realizing single-chemical-bond determination in surface chemistry, which can shed light on chemical identification and bond control of extensive carbon-based nanostructures/nanomaterials, and open up opportunities for further property optimization.

(5) Photoelectric conversion in single molecule on surface

Carrier generation induced by the light irradiation plays a significant role in various photoelectric conversion processes such as solar cell, photocatalyst, and photosynthesis. Detailed analyses of the photocurrent generation at the single-molecule level will contribute to the fundamental understanding of energy conversion and the development of novel functional materials for organic (opto)electronic devices. With recent progresses in experimental techniques of nanofabrication and optical measurements at nanoscale, it becomes possible to observe optical response in single molecule junctions. This gives rise to a new field of nanoscale research, named molecule optoelectronics.

In this work, we observe photocurrent generation in single molecule using a scanning tunneling microscope (STM) combined with a laser excitation. The dependence of photocurrent flux on the STM tip position and the applied bias voltage were measured for a free-base phthalocyanine (FBPc) molecule adsorbed on a three-monolayer thick NaCl film grown on a silver surface. To analyze the detailed mechanism behind the carrier generation dynamics, we conducted the theoretical analyses on the photocurrent generation processes. We formulated the current flux using Hubbard nonequiribrium Green function (NEGF) method, which has been developed by us recently. In this technique, the molecule-electrode coupling and molecule-radiative field coupling are taken into account within proper diagrammatic perturbation series expansion, which enables to analyze the dynamics of system beyond the Markov approximation. In the previous studies, it has been demonstrated that the technique is appreciable over the wide range of parameters. To conduct the system specific analysis, we performed first-principles calculations based on the density function theory (DFT) and time-dependent DFT (TDDFT) to extract the information of electronic and vibrational structure of the molecule. Other necessary parameters were quantitatively estimated based on the previous literatures.

Figure 8 shows the computational results for the photocurrent I_{ph} as a function of the applied bias voltage V_{bias} with the different position of the STM tip. The results are in good agreement of the experimentally observed data. At $V_{\mathrm{bias}} = 0$ V, the photocurrent shows positive value, where the electrons flow in the direction from the STM tip to the substrate. The steep decrease near -0.2 V is attributed to the opening of the conductance channel through the lowest unoccupied molecular orbital (LUMO) of the electrically excited FBPc molecule. We also reveal the mechanism behind the tip position dependence of I_{ph}, which can explain the spatial distribution of the photocurrent. The obtained knowledge would provide a fundamental understanding of the photoelectronic conversion processes at the molecule/substrate interfaces and a novel perspective for improving the energy conversion efficiency of organic (opto)electronic devices with the atomic-scale engineering.

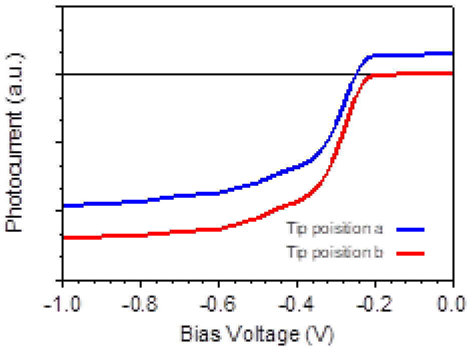

Figure 8. Computational results for the photocurrent I_{ph} as a function of the applied bias voltage V_{bias} with the different position of the STM tip.

4. Conclusion

We have tried to examine a variety of molecular behaviors on the surface in FY2020. Our theoretical studies combined with experiments in FY2020 provide deep insight into a variety of chemical and physical phenomena on solid surface: (1) Photochemistry and plasmon-induced chemical reactions, (2) Electron-phonon coupling at surface and interfaces, (3) Raman spectra of self-assembled monolayers on gold electrode, (4) Single molecule electroluminescence induced by the metal-molecule charge transfer. We expect that our results can provide new perspective to develop a potential strategy for controlling electronic properties of molecular adsorbates on the surface.

5. Schedule and prospect for the future

(1) Controlling chemical reactivity of ultrathin oxide film

Ultrathin oxide film grown on metal substrate has been a subject of great interest not only as a supporting material for chemically active nanoparticles but also as a catalyst in the field of heterogeneous catalysis, where it provides various ways to control the properties of adsorbates via following factors: (i) charge transfer between adsorbates and oxide-metal interface, which is closely correlated with the electronic affinity (EA) of adsorbate and work function reduction, (ii) adhesion between oxide and metal layers with strong polaronic distortion, (iii) film thickness, and (iv) the chemical composition of oxide surface. Therefore, we will continue our work to find the way for controlling the chemical reactivity using theoretical and experimental studies. In FY2021, we will extend our study into dissociation of OCS on MgO/Ag(100) using combined STM and DFT methodology. The influence from solvent medium on the chemical reactions occurring on surface will be studied in order to provide insights into the electrochemical reactions. In particular, regarding the OCS dissociation on MgO/Ag(100), we will try to find a way to selectively dissociate a bond in OCS, e.g., C-S, and C-O, using an ionic species on MgO film surface which is introduced through charge transfer between the oxide surface and oxide-metal interface. The other branch of our study is exploring the single atom catalyst on ultrathin oxide film, which is now widely studied due to its prominent importance in heterogeneous catalyst. Therefore, we will introduce single atom catalyst to oxide film and will study how to control its catalytic activity and selectivity. In addition, we are extending our model system to other ultrathin oxide film systems, such as titania and ceria. In FY2021, the study on titania will be intensively performed to find a proper supporting substrate to efficiently realize ultrathin titania film. We believe that our study provides not only profound insight into the chemical reactivity control of ultrathin oxide film but also an impetus for investigating ultrathin oxide films for a wider range of applications.

(2) Molecular adsorption on solid surface: From single molecule to molecular network, and their optical properties

The controllable fabrication of molecular architectures is a topic of great importance not only as a fundamental subject in surface science but also for realizing molecular-scale electronic devices. Computational techniques can provide the underlying mechanisms for the formation of various molecular architectures experimentally observed by STM as well as single molecule adsorption. For the adsorption of single molecules on metal substrate, we suggested the origin of adsorption-induced stability reversal of photochromic DAE on metal surfaces and revealed that the interfacial orbital interaction originated from the weak electronic coupling between the molecular π-state and the electronic states of the Au surface can play a decisive role in constraining adsorption geometry even in the archetypal vdW adsorption system. For one-dimensional (1-D) systems, we have explained (i) the formation mechanism of 1D zipper-type architecture of azobenzene derivatives with the balanced non-bonding interactions, H-bonding and vdW interactions, between adjacent molecules and (ii) the dispersive electronic feature due to the π-orbitals stacking in 1-D molecular lines fabricated on the Si(001)-(2×1)-H. For 2D systems, we contributed to unveil the adsorption geometry of 2D molecular films composed of fluorinated fullerene ($C_{60}F_{36}$), which is strongly related to the distribution of frontier molecular orbitals and thus the n-type character of molecular film. In addition, we revealed the novel formation mechanism of supramolecular assembly using photochromic diarylethene derivative, which is the first report on molecular architectures formed by ion-dipole interaction on solid surface. Very recently, the electronic structures of dimethyl disulfide (DMDS) adsorbed on Ag(111) and Cu(111) were also investigated for studying its photodissociation and plasmon induced chemical reaction on the surface. Our results provide not only deeper insight into the molecular adsorption process, but also a general basis for designing the architectures of molecular electronics with desired electronic properties. In FY2021, we will continue the research not only for a variety of molecular assemblies but also isolated molecule on the surfaces as follows: (1) the formation mechanism of van der Waals interface between π-conjugated molecule and novel metal substrate, and (2) optical property of adsorbate on solid surface, especially, O_2 dissociation on Ag(110) is now actively being studied.

(3) Electronic structures of layered materials, such as graphene and dichalcogenide, and of framework materials, such as MOF and COF

Electronic structures of layered materials, such as graphene and dichalcogenide, and of framework materials, such as MOF and COF. Functionalization of layered materials, such as graphene and dichalcogenide, has attracted great scientific interest not only in controlling their physical properties but also in improving chemical adaptability to integrate them as a building block into a variety of functional devices. In particular, we first suggested that the atomic oxidation of graphene grown on a metal substrate results in the formation of graphene enolate, i.e., negatively charged oxygen adsorbed at ontop position on its basal plane, which is strikingly different from the formation of epoxy groups, i.e., adsorption of atomic oxygen at bridge position, on pristine graphene and on graphite. Whereas the enolate is the transition state between two nearest epoxides both on graphene and on graphite, we revealed that improved interfacial interaction between graphene and metal substrate during atomic oxidation plays a crucial role not only in the formation of graphene enolate as a local minimum but also in stabilizing it over the graphene epoxide. In addition, we recently studied the growth mechanism of covalent organic framework (COF) through photo-excitation. In FY2021, we are going to theoretically investigate (1) our very recent experimental finding of well-ordered graphene functionalization with OH group, in which the formation of graphene enolate would be one of the main driving forces, and (2) the catalytic effect of metal-organic framework (MOF).

(4) Raman spectra of self-assembled monolayers on gold electrode

As mentioned in the above section, we have established the simulation method of Raman spectra for organic monolayers of metal surfaces. We will try to perform experiments for next half year, and will perform DFT calculation to find next more attractive targets.

(5) On-surface photo-induced reactions and syntheses

We have been trying to combine the theoretical calculations with STM/STS and TERS experiments to examine a variety of molecular behaviors and reaction pathways towards target nanostructures on the metal surfaces. Such kinds of study made a good combination of real-space observation and theoretical prediction to provide fundamental understandings into the underlying mechanisms in the on-surface reaction/self-assembly processes on the surfaces. In FY2021, we plan to further deeply explore some other topics related to the on-surface photo-induced synthesis from the following prospects: (1) adsorption configurations; (2) molecule-molecule interactions and molecule-substrate interactions; (3) electronic and magnetic properties; (4) possible reaction pathways.

(6) Photoelectric conversion in single molecule on surface

Our studies on carrier dynamics in energy conversion processes are extended to the research on photoelectric conversion in single molecule. Single molecule luminescence and photocurrent generation in single molecule under the light irradiation can be investigated with the aid of STM and optical measurements, enabling us to investigate the energy conversion processes with submolecular spatial resolution in a well-defined manner. Especially, we focus on electron correlations in these processes, e.g., charging of the molecule, formation of single/triplet excitons, radiative and nonradiative decay, and so forth. The key factor in the theoretical analysis is the calculation of (i) excited electronic states of the molecule as well as (ii) nonequilibrium electron dynamics under applied bias and/or light irradiation. We plan to investigate these points using the method based on first-principles calculations and the nonequilibrium Green’s function (NEGF) methods. Our study would make a contribution for understanding the fundamental nature of molecular energy conversion and in the designing of novel functional materials for organic (opto)electronic devices.

6. If no job was executed, specify the reason.

Usage Report for Fiscal Year 2020

Fiscal Year 2020 List of Publications Resulting from the Use of the supercomputer

[Paper accepted by a journal]

1. Rafael B. Jaculbia, Hiroshi Imada, Kuniyuki Miwa, Takeshi Iwasa, Masato Takenaka, Bo Yang, Emiko Kazuma, Norihiko Hayazawa, Tetsuya Taketsugu and Yousoo Kim, “Single-molecule resonance Raman effect in a plasmonic nanocavity”, Nat. Nanotechnol., 15, 105, (January, 2020)
2. Hyunseob Lim, Younghee Park, Minhui Lee, Jong-Guk Ahn, Bao-Wen Li, Da Luo, Jaehoon Jung, Rodney Ruoff and Yousoo Kim, “Centimeter-scale and highly crystalline 2D alcohol: evidence for graphenol (C_6OH)”, Nano Lett., 20, 2107 (February, 2020)
3. Jong-Guk Ahn, Jiwon Bang, Jaehoon Jung, Yousoo Kim, and Hyunseob Lim, “Scanning tunneling microscopic investigations for studying conformational change of underlying Cu(111) and Ni(111) during graphene growth”, Surf. Sci. 693, 121526 (March, 2020)
4. Emiko Kazuma, Minhui Lee, Jaehoon Jung, Michael Trenary and Yousoo Kim, “Single-molecule study of a plasmon-induced reaction for a strongly chemisorbed molecule”, Angew. Chem. Int. Ed., 59, 7960 (March, 2020)
5. Younghee Park, Seunghyun Shin, Young-Joon An, Jong-Guk Ahn, Geumbi Shin, Chaehyeon Ahn, Jiwon Bang, Jaeyoon Baik, Yousoo Kim, Jaehoon Jung and Hyunseob Lim, “Tunable optical transition in 2H-MoS_2 via direct electrochemical engineering of vacancy defect and surface S-C bond”, ACS Appl. Mater. Interfaces, 12, 40870 (August, 2020)

[Conference Proceedings]

[Oral presentation]

1. 數間恵弥子, “Nanoscale analysis and control of chemical reactions induced by localized surface plasmon”, 日本化学会第 100 春季年会(2020), 千葉県野田市, 3 月 23 日 (2020)
2. 數間恵弥子, “光 STM を用いたプラズモン誘起化学反応の単一分子レベル解析”, 表面真空学会関東支部の講演会, 慶應義塾大学日吉キャンパス, 神奈川県横浜市, 4 月 11 日 (2020)
3. 數間恵弥子, “プラズモンが誘起する単一分子化学反応の実空間観測”, JST ・触媒学会共催オンライン公開シンポジウム - 革新的触媒と反応制御の今後 - , YouTube 生配信 (https://bit.ly/2zn5eRM), 5 月 22 日 (2020)
4. E. Kazuma, M. Lee, J. Jung, M. Trenary, Y. Kim, “Single-molecule study of the plasmon-Induced dissociation of O_2 molecules”, The 5th International Workshop on Advanced Nanoscience and Nanomaterials 2020 (5th IWANN2020), Online, Oct. (2020)
5. 數間恵弥子, “単一分子プラズモン誘起解離反応の光 STM 観測・解析,”, ACE Meeting Online II, オンライン, 11 月 21 日 (2020)
6. 數間恵弥子, “単一酸素分子のプラズモン誘起解離反応の実空間観測”, 分子研研究会「ナノ空間で光が織りなす分子操作・化学反応制御の新展開」, オンライン, 12 月 4 日 (2020)

[Poster presentation]

[Others (Book, Press release, etc.)]