Computational Molecular Science Research Team

1. Team members

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2. Research Activities

Developing a Molecular Theory and Software for Predicting Reactions and Properties of Molecules

2.1. Original molecular science theory to explore new materials and drugs

An atomic- and molecular-level understanding of drug actions and the mechanisms of a variety of chemical reactions will provide insight for developing new drugs and materials. Although a number of diverse experimental methods have been developed, it still remains difficult to investigate the state of complex molecules and to follow chemical reactions in detail. Therefore, a theoretical molecular science that can predict the properties and functions of matter at the atomic and molecular levels by means of molecular theoretical calculations is keenly awaited as a replacement for experiment. Theoretical molecular science has recently made great strides due to progress in molecular theory and computer development. However, it is still unsatisfactory for practical applications. Consequently, our main goal is to realize an updated theoretical molecular science by developing a molecular theory and calculation methods to handle large complex molecules with high precision under a variety of conditions. To achieve our aim, we have so far developed several methods of calculation. Examples include a way for resolving a significant problem facing conventional methods of calculation, in which the calculation volume increases dramatically when dealing with larger molecules; a way for improving the precision of calculations in molecular simulations; and a way for high-precision calculation of the properties of molecules containing heavy atoms such as metal atoms.

2.2. New molecular science software NTChem

Quantum chemistry software comprises immensely useful tools in material and biological science

research. Widely diverse programs have been developed in Western countries as Japan has lagged. In fact, only a few programs have been developed in Japan. The mission of our research team is to provide K computer users with a high-performance software for quantum molecular simulation. In the early stage of the K computer project, no quantum chemistry software was available for general purpose and massively parallel computation on the K computer because not every program was designed for use on it. Therefore, we have chosen to develop a new comprehensive ab initio quantum chemistry software locally: NTChem. NTChem is completely new software that implements not only standard quantum chemistry approaches, but also original and improved theoretical methods that we have developed in our research work. The main features of the current version, NTChem2013, are the following:

1) Electronic structure calculation of the ground state of atoms and molecules based on Hartree–Fock (HF) and density functional theory (DFT) methods.

2) Linear-scaling or low-scaling DFT: Gaussian and finite-element Coulomb (GFC) resolution-of-the-identity (RI) DFT, pseudospectral DFT/HF, and dual-level DFT.

3) Low-scaling SCF calculation using diagonalization-free approaches: purification density matrix, pseudo-diagonalization, and quadratic convergence SCF.

4) Excited-state DFT calculation: time-dependent DFT (TDDFT) and transition potential (DFT-TP).

5) Accurate electron correlation methods for ground and excited states: Møller–Plesset perturbation theory, coupled-cluster (CC) theory, and quantum Monte Carlo (QMC) method.

6) Massively parallel computing on the K computer and Intel-based architectures: HF, DFT, resolution-of-the-identity second-order Møller–Plesset (RI-MP2) method, and QMC method.

7) Two-component relativistic electronic structure calculation with spin–orbit interactions: Douglas–Kroll (DK) (DK1, DK2, and DK3), regular approximation (RA) (zeroth-order RA (ZORA) and infinite-order RA (IORA)), and Relativistic scheme for Eliminating Small Components (RESC).

8) Model calculations for large molecular systems: quantum mechanics/molecular mechanics (QM/MM) and Our own N-layered Integrated molecular Orbital and molecular Mechanics (ONIOM).

9) Calculation of solvation effects: COnductor-like Screening MOdel (COSMO) (interfaced with the HONDO program), averaged solvent electrostatic potential/molecular dynamics (ASEP/MD), and QM/MM-MD.

10) Efficient calculation for chemical reaction pathway.

11) Ab initio molecular dynamics calculation.

12) Calculation of magnetic properties: nuclear magnetic resonance (NMR) chemical shifts, magnetizabilities, and electron paramagnetic resonance (EPR) g tensors.

13) Population analysis: Mulliken and natural bond orbital (NBO) analysis (interfaced with NBO 6.0).

14) Orbital interaction analysis: maximally interacting orbital (MIO) and paired interacting orbital (PIO) methods.

3. Research Results and Achievements

3.1. Development of massively parallel algorithm of RI-MP2 energy calculation and RI-MP2 analytical energy gradient calculation on peta-flops supercomputers

Second-order Møller–Plesset perturbation (MP2) theory is the simplest but robust electron correlation method to account for the non-covalent interactions that play important roles in the chemical phenomena of nano and biological molecules. In our previous study, we developed the MPI/OpenMP hybrid parallel algorithm (J. Chem. Theory Comput. 9, 5373 (2013)) for the resolution of the identity MP2 (RI-MP2) energy calculation of nano-scale molecules on peta-flops supercomputers and implemented into the NTChem software. However, it was difficult to perform the RI-MP2 calculations more than 10,000 MPI processes on the peta-scale supercomputers using the previously reported algorithm because it had the limitation of the available MPI processes.

We have developed the improved version of the MPI/OpenMP hybrid parallel algorithm for the RI-MP2 energy calculations. In this algorithm, we have developed the dual-level parallelization scheme to utilize more than 10,000 MPI processes on the peta-scale supercomputers such as the K computer and TSUBAME 2.5. We have also devised the network communication scheme overlapping the computation and the network communication during the evaluation of four-center two-electron repulsion integrals to reduce the overhead and the latency of network communication. We checked the scalability of parallel algorithm performing test calculations of nanographene stacked dimer $(C_{150}H_{30})_2$ at the RI-MP2/cc-pVTZ level (9,840 atomic orbitals (AOs) without the frozen core approximation) using up to 80,199 nodes of the K computer. The parallel performance scales up to the 80,199 nodes and the 3.1 peta FLoating OPerations per second (FLOPs) of peak performance has been attained using 80,199 nodes. We have performed the multi-node and multi-graphic processing unit (GPU) implementation based on the present algorithm. The DGEMM matrix–matrix multiplication during the RI-MP2 calculation is offloaded to the GPU devices. The dual-level parallelization scheme is also suitable for utilizing the multi-nodes and multi-GPUs where the computation of sub-matrices is assigned to each GPUs. Considerable speedups of the RI-MP2 calculation can be attained by the present multi-node and multi-GPU implementation. The peak performance of the central processing unit (CPU) computation and the CPU/GPU hybrid computation of nanographene stacked dimer $(C_{96}H_{24})_2$ (9,840 atomic orbitals (AOs) without the frozen core approximation) using 1,349 nodes and 4,047 GPUs of TSUBAME 2.5 are 87.5 tera FLOPs and 514.7 tera FLOPs, respectively.

In the case of geometry optimization, the MP2 analytical energy gradient calculation is more demanding than the MP2 energy calculation because of the high computational cost with very large

prefactors. Thus, the efficient computational algorithm and implementation for the MP2 energy gradient is desired. We have developed an MPI/OpenMP hybrid parallel algorithm for the RI-MP2 energy gradient calculation of nano-scale molecules and implemented into the NTChem software. This algorithm is designed for the massively parallel calculations on the peta-flop supercomputers such as the K computer. The loop of a virtual molecular orbital index is parallelized by MPI in the calculation of two-electron integrals, one-particle density matrices, and two-particle density matrices to utilize more than a few thousand MPI processes. The dual-level parallelization scheme and the network communication scheme overlapping the computation and network communication mentioned above have also been applied to the RI-MP2 energy gradient algorithm. The RI-MP2/cc-pVTZ energy gradient calculation of buckycatcher $C_{60}@C_{60}H_{28}$ (3,992 AOs without the frozen core approximation) was successfully performed in 30 minutes using 4,096 nodes of the K computer. Using the new MPI/OpenMP hybrid parallel RI-MP2 energy gradient code, the MP2 geometry optimization of large molecules having up to 200 atoms and 5,000 AOs can be performed with high parallel performance and in modest time on the K computer.

3.2. Development of higher-order time-dependent density functional theory for nonlinear optical properties

Molecular materials exhibiting large second-order nonlinear optical (NLO) responses have received increasing interest in recent years, experimentally as well as theoretically owing to their applicability in fields such as noninvasive imaging, three-dimensional optical data storage and optical power limiting. Correct description of excited states involved in NLO responses frequently requires inclusion of the higher order electronic correlations. This makes their computing a much more complicated procedure compared to analogous ground state calculations. Recently, time-dependent density functional theory (TDDFT) has emerged as an accurate and efficient method for studying the optical response of molecules. Including the electron correlation through the exchange–correlation functional, excellent results have been obtained for organic molecules, organometallic compounds, inorganic finite clusters, and infinite crystals.

In this work, we have implemented dynamic linear-, quadratic-, and cubic-response TDDFT method for nonlinear optical response of molecules in the NTChem program. The implemented code can calculate the typical nonlinear optical properties such as electrooptic Pockels effect (EOPE), second harmonic generation (SHG), optical rec- tification (OR), DC-electric field induced (EFI)SHG, third harmonic generation (THG), optical Kerr effect (OKE), and intensity dependent refractive index (IDRI). Those implementations closely follow the algorithm presented by Sekino and Bartlett for higher-order time-dependent Hartree–Fock theory. Higher-order Kohn–Sham matrices of higher-order Kohn–Sham equations require higher-order functional derivatives of the exchange–correlation functionals, which have been derived and implemented into efficient computer codes

with the aid of a computerized symbolic algebra system.

3.3. Development of screened Hartree–Fock exchange potential using position-dependent atomic dielectric constants

Screening effects on the exchange potential have been gathering a lot of attentions in first-principles band structure calculations. The importance of the screened exchange term has been discussed in the GW method and the COHSEX approximation, which was proposed by Hedin in 1965. One of important characteristics of the GW method is to improve the bandgap property of semiconductors, although the local density approximation (LDA) of density functional theory (DFT) underestimates the bandgap due to the lack of nonlocal exchange interactions. In the static COHSEX approximation of the GW method, electron correlation effects related to the random phase approximation (RPA) are divided into two contributions of the Coulomb-hole (COH) and the screened exchange (SEX) interactions. The non-local SEX contribution is essential to improve the bandgap problem of the LDA method. The hybrid DFT functionals which possess a partial Hartree–Fock (HF) exchange term can also give better agreements between calculations and experiments. Thus, the GW and hybrid-DFT methods can provide good solutions for the bandgap problem. Several studies have pointed out theoretical relationships between the GW method and the hybrid-DFT functionals. We developed a dielectric-dependent screened HF exchange potential approach and the dielectric-dependent Slater-formula and COH interaction. In the dielectric-dependent screened exchange approach, the ratio of the HF exchange term mixed into screened exchange potential is proportional to the inverse of the dielectric constant. In addition, we studied the screened HF exchange potential using position-dependent atomic dielectric constants. The estimations of the atomic dielectric constant are incorporated into the SCF loop, and those values are automatically determined in each SCF step. In order to confirm the adequacy of our position-dependent methodology, the energy band structures of several semiconductors are calculated, and the position-dependent approach can give good agreements with experimental results.

3.4. Development of computational scheme for natural circular dichroism

When lights have different degrees of circular polarization, they are absorbed differently by optically active chiral molecules. With no external magnetic field, this effect is called natural circular dichroism. Experimental circular dichroism spectroscopy has widely been used as a powerful tool to investigate structure of large molecules including protein, because of its sensitivity to the molecular conformation. In NTChem, we have implemented a functionality to investigate this natural circular dichroism, associated with electronic state excitations. In our implementation, both scalar and tensor rotational strength can be calculated in length or velocity representation. The conventional scalar rotational strength is relevant for light absorption by randomly oriented molecules, e.g., in gas-phase

or in solvent, whereas the tensor rotational strength is relevant for light absorption by oriented molecules, e.g., molecules adsorbed on surface. This new functionality is expected to be valuable calculational tool to interpret experimental results in circular dichroism spectroscopy.

3.5. Development of utility program for QM/MM combined calculation

For large systems such as proteins and supramolecules, fully quantum mechanical (full-QM) calculations are still too costly and some approximate approaches are required. Such approximate methods which combine accurate QM and less demanding molecular mechanical (MM) calculations are important portion of the NTChem program. However, to prepare NTChem input file for such multilevel calculations such as QM/MM and ONIOM calculations, are complicated and cumbersome. Thus, we developed a utility program for preparing QM/MM combined methods, which enables users to prepare input files for QM/MM calculations by using standard Tinker input and parameter files and indicating QM atoms. This utility program is written in Fortran90 and placed in NTChem tools packages.

3.6. Implementation of parallel algorithm for sparse-matrix algebra toward large-scale calculation of quantum chemistry

Recent development of computers has been making it possible to perform predictive calculations of electronic systems containing large molecules. For such calculations, we should employ linear-scaling methods, which are mainly used in the calculations based on the density functional theory (DFT). One of the most efficient methods for obtaining the ground state of a large electronic system is the purification method, in which the many multiplications of large sparse matrices are performed until convergence. The most crucial factor is thus the use of computationally as less demanding algorithm as possible for the multiplication of large sparse matrices. A promising algorithm for sparse-matrix algebra was proposed recently, in which a large sparse matrix is distributed to processors according to the density of the nonzero elements in the matrix and the multiplication between such matrices are efficiently performed using the communication. Specifically, a large matrix is divided into submatrices and their sparsity are determined in advance of multiplication. If the sparsity of two submatrices involved in the multiplication is dense, the ordinary matrix multiplication is performed. Otherwise, only the nonzero elements in the submatrices are sent and received for the multiplication. This treatment reduces the amount of data in the communications.

3.7. Theoretical design of dye sensitizers by two-component relativistic time-dependent density functional theory with spin–orbit interaction

Ru complexes have been demonstrated as a promising dye among solar cell materials. Recently, a

phosphine-coordinated Ru(II) sensitizer, DX1 molecule, was reported to perform well as an organic photovoltaic material. The DX1 molecule has the feature that spin-forbidden singlet-to-triplet direct transitions occur because of the strong spin–orbit (SO) interaction, which indicates that the DX1 sensitizer can absorb long-wavelength lights through the spin-forbidden transitions. Last year, we successfully reproduced the spin-forbidden transitions by two-component relativistic time-dependent density functional theory/ Tamm–Dancoff approximation with the SO interaction (2c-TDDFT/TDA), which was implemented into NTChem. This year, we newly examined the roles of the central transition metal by replacing Ru with Fe and Os. The numerical investigation reveals that the absorption spectrum of DX1–Fe is similar to that of DX1–Os but is significantly different. DX1–Os can absorb longer wavelength light with relatively small oscillator strengths in comparison with DX1, whereas DX1–Fe cannot. This investigation provides information about the roles of transition metals in dye sensitizers, which would be useful for constructing new sensitizers using spin-forbidden transitions.

3.8. Computational application to organic photovoltaics

Compared to the conventional silicon-based solar cells, organic photovoltaics (OPV) are characterized by their lower production costs, lower weights and greater flexibilities. In addition, OPV can be produced by printing on materials so that they are expected to be useful for electric power generation on complex shaped materials like household goods, furniture, textile, and so on. Despite significant research efforts, detailed understanding of microscopic processes in OPV is still lacking. Especially, the charge generation mechanism at the heterojunction between donor and acceptor has been debated for a while. To understand this process, we have investigated the properties excited electronic states in a P3HT:PCBM monomer pair, where P3HT is a popular donor polymer material and PCBM is an acceptor material derived from C_{60} fullerene, using the time-dependent DFT method. We calculated the electronic couplings for charge separation from the exciton at a P3HT monomer, and recombination from charge transfer state to the ground electronic state.

3.9. A computational estimation for orbital energies of polymer toward the development of organic photovoltaic cells

We theoretically investigated physical properties including orbital energies and excitation energies of frontier orbitals for the multifunctional thiophene-based polymers composed of donor- and acceptor-units. Orbital analysis reveals that the remarkably different behavior of frontier orbital energies with respect to the degree of the polymerization stems from the distributions of frontier orbitals, which is insightful information for controlling ionization potentials and electron affinities of multifunctional polymers. We also estimated frontier orbital energies of the polymers through a

simple Hückel-theory based analytical model parameterized from calculations of relatively small oligomers. In this model, we set two parameters: one is the orbital energy of each monomer α and the other is interaction energy corresponding to the resonance integral ß. Assumed that the resonance integral ß is proportional to the density of the edge atom connected to the next monomer, the orbital energy of a polymer can be estimated by its monomer. By using the fitted parameter, the estimated value from the data of a monomer can reproduce the orbital energy of the polymer. These analyses are meaningful for a future design of thiophene-based polymers for solar cell materials; for instance, we can design a new polymer that absorbs important long wavelength sunlight so that the LUMO energies decrease with respect to the degree of the polymerization by controlling orbital energies of the donor and acceptor units in the polymer.

4. Schedule and Future Plan

In the next financial year, we will develop the new algorithm and improve the parallel efficiency of the NTChem2013 suit of program. In addition, we will make NTChem more user-friendly. Currently, NTChem is available on several cluster and supercomputer systems (the supercomputer system of Research Center for Computational Science at the Institute for Molecular Science and the supercomputer system of the Foundation for Computational Science) as well as the K computer. In the near future, we hope to make NTChem available to the general public. We intend to continue adopting users' requests with the aim of making the program more convenient and user-friendly for researchers in various fields. We earnestly hope that NTChem will be an important tool leading the way toward a new frontier of computational molecular science.

5. Publication, Presentation and Deliverables

(1) Journal Papers

1. T. Nakajima, M. Katouda, M. Kamiya, Y. Nakatsuka, "NTChem: A high-performance software package for quantum molecular simulation", Int. J. Quantum Chem. 115, 349–359 (2015).

2. T. Nakajima, "Molecular science software "NTChem" and its application to complex systems", in Quantum and computational chemistry for metal complex systems (2014). (in Japanese)

3. T. Nakajima, "Douglas–Kroll method", Journal of Computer Chemistry, Japan, 13, 50‑70 (2014). (in Japanese)

4. T. Shimazaki, T. Nakajima, "Theoretical study of a screened Hartree-Fock exchange potential using position-dependent atomic dielectric constants", J. Chem. Phys., 142, 074109 (2015).

5. M. Shoji, H. Isobe, S. Yamanaka, Y. Umena, K. Kawakami, N. Kamiya, J.-R. Shen, T.

Nakajima, K. Yamaguchi, "Large Scale QM/MM Calculations of Oxygen Evolving Complex of Photosystem II. Elucidation of Hydrogen Bonding Networks for Proton Transfer and Water Inlet Channels for Water Oxidation", Advances in Quantum Chemistry, 70, 325–413 (2015).

6. Y. Ootani, Y. Akinaga, T. Nakajima, "Theoretical Investigation of Enantioselectivity of Cage-Like Supramolecular Assembly: The Insights into the Shape Complementarity and Host–Guest Interaction", J. Comput. Chem. 36, 459–466 (2015).

7. M. Shoji, H. Isobe, S. Yamanaka, Y. Umena, K. Kawakami, N. Kamiya, J.-R. Shen, T. Nakajima, K. Yamaguchi, "Theoretical modelling of biomolecular systems I. Large-scale QM/MM calculations of hydrogen-bonding networks of the oxygen evolving complex of photosystem II", Mol. Phys. 113, 359–384 (2015).

8. K. Sugahara, N. Satake, K. Kamata, T. Nakajima, N. Mizuno, "A Basic –7-Charged Germanodecatungstate Efficient for Chemoselective Acylation of Primary Alcohols", Angew. Chem. Int. Ed. 126, 13464–13468 (2014).

9. T. Shimazaki, T. Nakajima, "Dielectric-dependent screened Hartree-Fock exchange potential and Slater-formula with Coulomb-hole interaction for energy band structure calculations", J. Chem. Phys. 141, 114109 (2014).

10. K. Uehara, T. Miyachi, T. Nakajima, N. Mizuno, "Effects of heteroatoms on electronic states of divanadium-substituted γ-Keggin-type polyoxometalates", Inorg. Chem. 53, 3907–3918 (2014).

11. T. Shimazaki, T. Kosugi, T. Nakajima, "Range-Separation Density-Fitting Band Structure Calculation with Gaussian Auxiliary Function", J. Phys. Soc. Jan, 83, 054702 (6 Pages) (2014).

12. R. Sakanoi, T. Shimazaki, J. Xu, Y. Higuchi, N. Ozawa, K. Sato, T. Hashida, M. Kubo, "Different Behavior of Young's Modulus and Fracture Strength of CeO2: Density Functional Calculation", J. Chem. Phys., 140, 121102 (2014).

13. Y. Ikabata, Y. Tsukamoto, Y. Imamura, H. Nakai, "Local Response Dispersion Method in Periodic Systems: Implementation and Assessment", J. Comput. Chem. 36, 303–311 (2015).

14. Y. Imamura, K. Suzuki, T. Iizuka, H. Nakai, "Linearity Condition for Orbital Energies in Density Functional Theory (V): Extension to Excited State Calculations", Chem. Phys. Lett. 618, 30–36 (2015).

15. T. Baba, T. Matsui, K. Kamiya, M. Nakano, Y. Shigeta, "A density functional study on pKa of small polyprotic molecule", International Journal of Quantum Chemistry, 114, 1128–1134 (2014).

(2)   Conference Papers

(3)   Invited Talks

1.   T. Nakajima, "Catalysis design with NTChem", 6th ESICB symposium, Tokyo, 18 March 2015. (in Japanese)

2.   T. Nakajima, "Development of application software and co-design in post-K project", 1st ft-energy symposium, Okazaki, 10 March 2015 (in Japanese)

3.   T. Nakajima, "Molecular science software "NTChem" and drug design", 2014 drug design informatics seminar, Tokyo, 17 December 2014 (in Japanese)

4.   T. Nakajima, "Molecular science software "NTChem"", VINAS Users Conference 2014, Tokyo, 10 October 2014. (in Japanese)

5.   T. Nakajima, "Simulation for organic film solar cell and photosynthesis", 2nd TCCI informal meeting, Nagoya, 27 September 2014 (in Japanese)

6.   T. Nakajima, "NTChem Program Package", Current Topics in Theoretical Chemistry, Nha Trang Workshop 2014, Nha Trang, Viet Nam, 25 Aug. 2014.

7.   T. Nakajima, "Post K project in AICS – molecular science –", Post K seminar, Okazaki, 1 April 2014. (in Japanese)

8.   M. Kamiya, T. Nakajima, "Development of Two-component Relativistic Time-dependent Density Functional Theory with Spin-orbit Interaction", Second China-Japan-Korea Tripartite Workshop on Theoretical and Computational Chemistry (CJK-WTCC-II), Kobe (Japan) 23 Jan. 2015.

9.   M. Katouda, "Algorithm and implementation of Møller–Plesset perturbation theory for petaflops supercomputers", 4th International Workshop on Massively Parallel Programming Now in Quantum Chemistry and Physics - Toward post-K computers, Tokyo, 24 Nov. 2014.

10.   T. Shimazaki, T. Nakajima, "Development of range-separation density-fitting approach for band structure calculations based on Gaussian basis set", 18th Malaysian International Chemical Congress, Kuala Lumpur, Malaysia, 3 Nov. 2014.

11.   Y. Imamura, "Theoretical Investigation on Dye Sensitizer Solar Cell: Spin-forbidden Transition", 11th International Conference of Computational Methods in Sciences and Engineering (ICCMSE 2015), Athens (Greece), 20 Mar. 2015.

12.   T. Matsui, "A novel computational scheme to estimate the redox potential of metal complex", The 64th Conference of Japan Society of Coordination Chemistry, Tokyo, Japan, 18 September 2014.

13.   M. Tashiro, "Molecular double core-hole state: theoretical analysis of photo- and Auger electron spectra", International Workshop "Atomic and molecular physics: a joint Japanese and French view over 120 years", Cernay la Ville France, 21–23 July 2014.

(4) Posters and presentations

1. T. Matsui, J.-W. Song, K. Hirao, T. Nakajima, "Computational Scheme for Redox Potential with Long-range Corrected Density Functional Theory", The 95th Annual meeting of Chemical Society of Japan, Funabashi, Japan, 29 March 2015.

2. M. Katouda, T. Nakajima, "Massively parallel RI-MP2 energy gradient algorithm for geometry optimization on petaflops supercomputers", International Workshop on New Frontier of Numerical Methods for Many-Body Correlations—Methodologies and Algorithms for Fermion Many-Body Problems, Tokyo, 20 Feb. 2015. (Poster)

3. M. Katouda, T. Nakajima, "Massively parallel RI-MP2 energy gradient calculations on K computer", 5th AICS International Symposium, Kobe, 8 Dec. 2014. (Poster)

4. M. Katouda, T. Nakajima, "MPI/OpenMP hybrid parallel algorithm of RI- MP2 energy gradient calculation for massively parallel multicore supercomputers", QSCP-XIX, Taipei, 13 Nov. 2014. (Poster)

5. Y. Imamura, M. Kamiya, T. Nakajima, "Theoretical Study on Solar Cell Sensitizers by Two-component Relativistic Time-dependent Density Functional Theory", the 19th International Workshop on Quantum Systems in Chemistry, Physics and Biology (QSCP-XIX), Taipei (Taiwan), 13 Nov. 2014.

6. M. Kamiya, H. Sekino, T. Nakajima, "Development of time-dependent density functional theory for frequency-dependent nonlinear optical response", 8th Annual Meeting of Japan Society for Molecular Science, Kyoto, Japan, 24 September, 2014. (Poster)

7. Y. Imamura, M. Kamiya, T. Nakajima, "Theoretical Study on Design for Efficient Dye Sensitized Solar Cell Materials", Annual Meeting of Japan Society for Molecular Science (2014), Higashi Hiroshima, 23 Sep. 2014.

8. Y. Imamura, M. Kamiya, T. Nakajima, "Theoretical Study on Photo Functional Materials by Two-component Relativistic Time-dependent Density Functional Theory", 17th Theoretical Chemistry Symposium, Nagoya, 23 May 2014.

(5) Patents and Deliverables