シンポジウム | アジア国際シンポジウム：アジア国際シンポジウム―物理化学ディビジョン／理論化学・情報化学・計算化学ディビジョン／分子科学会共催―

2026年3月17日(火) 13:00 ~ 15:40 | A1421（14号館 [2階] 1421）

[A1421-1pm] アジア国際シンポジウム―物理化学ディビジョン／理論化学・情報化学・計算化学ディビジョン／分子科学会共催―

座長，シンポジウム関係者：北河 康隆（大阪大学）、板倉 隆二（量子科学技術研究開発機構）、中井 浩巳（早稲田大学）、立川 仁典（横浜市立大学）、小林 正人（北海道大学）

本セッションは午後、夕刻に実施されます。

13:00 ~ 13:05
開会挨拶

英語 Invited Lecture
13:05 ~ 13:35
[A1421-1pm-01] Coherent vibrational spectroscopy and quantum optical femtosecond spectroscopy

○Kim JunWoo[1] (1.Chungbuk National University)

13:35 ~ 13:40
休憩

英語 Invited Lecture
13:40 ~ 14:00
[A1421-1pm-02] 量子もつれ光を光源とする蛍光寿命測定

○松崎 維信[1] (1.理化学研究所)

英語 Invited Lecture
14:00 ~ 14:20
[A1421-1pm-03] 強いパラメトリック増幅を用いた非検出光子による中赤外干渉計測

○橋本 和樹[1,2] (1.東京大学、2.マックスプランク光科学研究所)

14:20 ~ 14:25
休憩

英語 Asia Special Lecture
14:25 ~ 14:55
[A1421-1pm-04] Exploring Quantum Computing for Protein-Drug Binding Affinity Prediction

○Vannajan Sanghiran Lee[1], Ruzanna Yahya[1], Nizamuddin Mohammad Alinor[1] (1.Center of Excellence in Quantum Information Science and Technology (QIST), Department of Chemistry, Faculty of Science Universiti Malaya, Kuala Lumpur, Malaysia)

14:55 ~ 15:00
休憩

英語 Invited Lecture
15:00 ~ 15:20
[A1421-1pm-05] フラグメント分子軌道法による有機半導体材料の光物理過程の解析

○藤田 貴敏[1] (1.QST量子生命研)

英語 Invited Lecture

15:20 ~ 15:40

[A1421-1pm-06] 明示的溶媒を考慮した分子動力学シミュレーション

○村上 龍大[1] (1.東京都立大学)

Coherent vibrational spectroscopy and quantum optical femtosecond spectroscopy

([1]*Chungbuk National University*) ○JunWoo Kim[1]

Keywords: Time-resolved spectroscopy; Vibrational wavepacket; Reaction dynamics; Quantum optical spectroscopy

Femtosecond spectroscopy provides far more than ultrafast temporal resolution; it enables the direct observation of quantum vibrational and electronic dynamics involved in specific light–matter interactions through vibrational or electronic coherences. This presentation will cover two related topics. The first focuses on the identification of reaction-associated vibrational modes by analyzing vibrational coherences that appear in femtosecond time-resolved spectra. Vibrational modes that are coupled to or actively participate in a reaction pathway exhibit characteristic modulations in their coherence signals as the reaction proceeds. By examining the evolution of these coherence features, it becomes possible to pinpoint reactive vibrational modes and gain insight into the underlying reaction dynamics.[1]

Femtosecond spectroscopy has been widely applied not only to relatively simple molecular or solid-state systems, where theoretical assumptions allow significant simplification, but also to complex biological assemblies such as photosynthetic complexes. However, in such complex systems, selectively probing a desired light–matter interaction pathway remains highly challenging due to the presence of numerous competing processes. Quantum light sources offer unique advantages in this context, possessing properties such as particle-like behavior and quantum entanglement that are not accessible with classical light. The second part of this presentation will introduce our efforts to develop a quantum optical spectroscopy technique that utilizes quantum light to achieve enhanced pathway selectivity in light–matter interactions.[2] By exploiting the nonclassical characteristics of quantum light, this approach aims to isolate specific interaction channels that are otherwise obscured in conventional femtosecond spectroscopic measurements.

1) JW. Kim, D. Kang, S. K. Kim, T. Joo, *Phys. Chem. Chem. Phys*. **2020**, *22*, 25811-25818. 2) EH. Hong, ES. Jang, JW. Kim, *Sci. Adv*. **2025**, *11*, eadw9759.

Fluorescence Lifetime Measurement Using Entangled Photon Pairs as the Light Source

([1]*RIKEN Center for Advanced Photonics, RIKEN*, [2]*Molecular Spectroscopy Laboratory, RIKEN*) ○Korenobu Matsuzaki[1,2]

Keywords: Entangled Photon Pairs; Fluorescence Lifetime; Microscopy

Fluorescence lifetime is widely utilized for identifying fluorescent species as well as for examining the nanometer-scale local environment around fluorescent molecules. Fluorescence lifetime is usually measured using a pulsed laser as the light source, because it can photo-excite a sample at a well-defined instant, which makes it possible to evaluate how much the subsequent fluorescence emission is delayed from the photo-excitation. The use of a pulsed laser, however, poses several limitations to the measurements. First, the high peak intensity of the pulsed laser may cause damage to photo-labile samples. Second, a pulsed laser produces a large number of excited species simultaneously within the sample, which may cause unwanted interaction among excited species, obscuring the true optical response of the system. Thus, it is desirable to perform fluorescence lifetime measurements without using a pulsed laser.

To realize such measurements, we opted to use entangled photon pairs instead of a pulsed laser as the light source.[1] Entangled photon pairs are a nonclassical state of light, where every photon is paired with another photon. They can be generated based on spontaneous parametric down conversion (SPDC) by irradiating a continuous-wave (cw) laser onto a nonlinear crystal such as β-barium borate (BBO). In this process, a photon in the laser is split into two photons to become an entangled photon pair. Since those two paired photons are generated simultaneously, there is a temporal correlation between the two photons, which can be utilized to realize time-resolved measurements such as fluorescence lifetime measurements. In such measurements, the drawbacks arising from the use of pulsed lasers are completely avoidable, because the entangled photon pairs are generated using a cw laser.

Fig. 1 shows the experimental setup developed in this study to realize fluorescence lifetime measurements using entangled photon pairs as the light source. The entangled photon pairs were obtained by SPDC in BBO pumped by a cw laser at 261 nm. After rejecting the pump laser using a longpass filter at 355 nm, paired photons at 532 ± 9 nm and 513 ± 8 nm were separately obtained using a dichroic mirror and bandpass filters. Here, the two wavelengths were chosen by considering the wavelength correlation between the paired photons. The 513 ± 8 nm component was introduced into a homebuilt microscope and was focused onto a sample using an objective lens (NA 1.35, 40x). The fluorescence from the sample was collected using the same objective lens, separated from the excitation light by the combination of a shortpass dichroic mirror at 535 nm and a longpass filter at 532 nm, and then detected by an avalanche photodiode (APD). The 532 ± 9 nm component, on the

other hand, was directly detected by another APD and was used as a temporal reference.

Fluorescence lifetime was measured by evaluating the difference in the photon detection timing on the two APDs using a time-correlated single photon counting (TCSPC) apparatus.

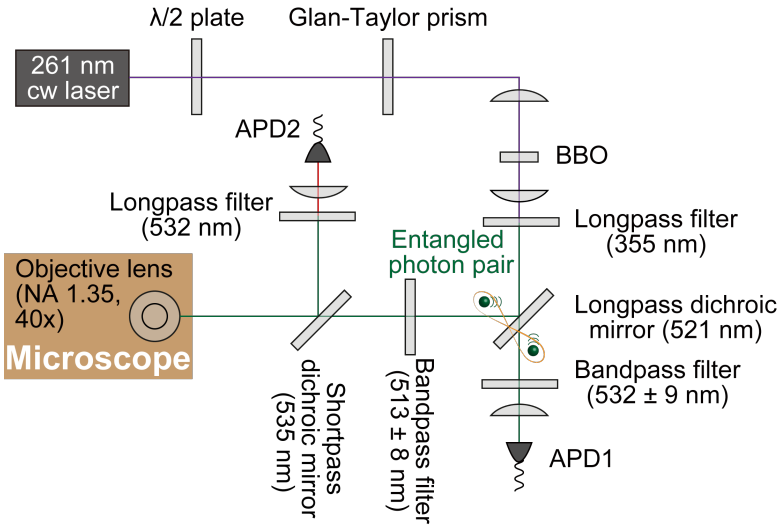

Figure 1. Schematic of the fluorescence lifetime measurement setup using entangled photon pairs as the light source.

Fig. 2 shows a fluorescence decay curve of rhodamine 6G embedded in poly(methyl methacrylate) (PMMA) measured by the apparatus shown in Fig. 1. By fitting the decay curve using a single exponential function convolved with a Gaussian function, which accounts for the instrumental response, the fluorescence lifetime was determined to be 4.2 ns. This result demonstrates that fluorescence lifetime measurements are indeed possible using entangled photon pairs instead of a pulsed laser.

While the measurement in Fig. 2 was done on a homogeneous sample, it is also possible to perform the same measurement on a heterogeneous sample in a spatially resolved manner, because the setup in Fig. 1 is constructed based on a microscope. In the presentation, we will discuss such spatially resolved fluorescence lifetime measurements using entangled photon pairs as the light source.

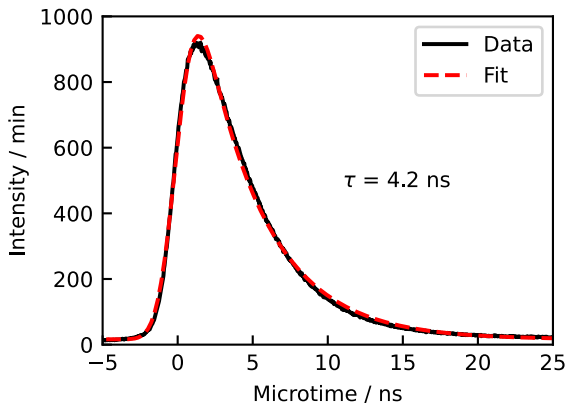

Figure 2. Fluorescence decay curve of rhodamine 6G in PMMA measured by using entangled photon pairs as the light source. A single exponential function convolved with a Gaussian function was used for the fitting analysis.

1) K. Matsuzaki, T. Tahara, and K. Ishii, Japanese patent No. 7636811 (priority date: Feb. 26, 2020; registration date: Feb. 18, 2025).

Mid-infrared interferometry with undetected photons via strong parametric amplification

([1]*Institute for Photon Science and Technology (IPST), The University of Tokyo*, [2]*Max Planck Institute for the Science of Light (MPL)*) ○Kazuki Hashimoto,[1,2]
Keywords: *Infrared Spectroscopy, Quantum Optics, Nonlinear interferometer*

Mid-infrared (MIR) spectroscopy and interferometry enable analysis of fundamental molecular vibrations and measurement of depth profiles in opaque (to visible (VIS)/near-infrared (NIR)) and scattering samples, respectively. However, MIR optical components, such as light sources and photodetectors, still exhibit inferior performance compared with their VIS/NIR counterparts. In particular, MIR photodetectors generally have lower sensitivity and higher noise, and additionally suffer from large thermal background noise.

Nonlinear interferometry based on nonlinear processes, such as spontaneous parametric down-conversion (SPDC), enables measurement of MIR transmittance and reflectance without directly detecting MIR (idler) radiation, instead by detecting VIS/NIR (signal) light. This "undetected photons" approach has been applied to MIR spectroscopy and low-coherence interferometry (LCI) by several research groups[1-4]. However, previous demonstrations have operated in the low-parametric-gain regime, where the mean photon number per mode is much smaller than one.

In this talk, I present the "undetected photons" technique implemented in the high-parametric-gain regime using intense-pulse excitation, which we carried out in Prof. Maria Chekhova's laboratory at Max Planck Institute for the Science of Light[5,6]. Parametric amplification in the nonlinear medium enables probing a sample with a relatively weak MIR idler while detecting the transmittance/reflectance with a strong VIS signal. Using the developed system, we measured broadband MIR absorption spectra of polymers and analyzed the depth profile of VIS-opaque reflective samples.

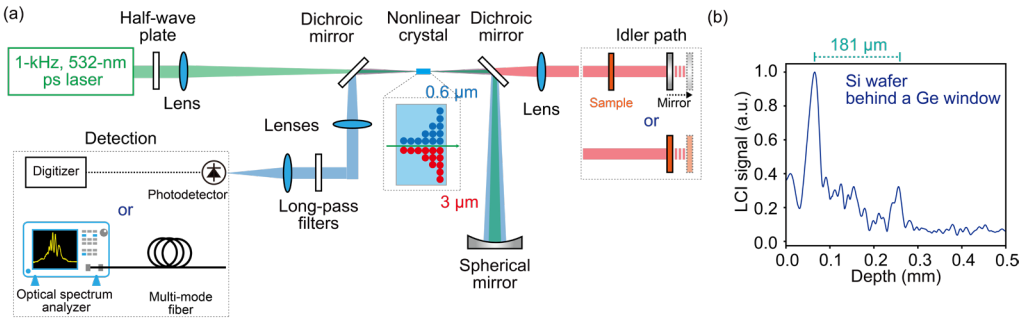

Fig. 1 (a) Schematic. (b) MIR-LCI of a Si wafer placed behind a Ge window.

1) D. A. Kalashnikov et al., *Nat. Photonics* **2016**, 10, 98. 2) C. Lindner et al., *Opt. Express* **2020**, 28, 4426. 3) T. Tashima et al., *Optica* **2024**, 11, 81. 4) A. Vanselow et al., *Optica* **2020**, 7, 1729. 5) K. Hashimoto et al., *Commun. Phys.* **2024**, 7, 217. 6) G. Zotti et al., *Opt. Lett.* **2025,** 50, 7636.

Exploring Quantum Computing for Protein-Drug Binding Affinity Prediction

([1]*Center of Excellence in Quantum Information Science and Technology, Department of Chemistry, Faculty of Science, Universiti Malaya, 50603 Kuala Lumpur Malaysia*) ○ Vannajan Sanghiran Lee,[1] Ruzanna Yahya,[1] Nizamuddin Mohammad Alinor[1]

Keywords: Quantum Computing, Quantum Machine Learning (QML), Protein–Drug Binding Affinity, Protein–Ligand Interaction, Drug Discovery

The prediction of molecular binding activity remains a central bottleneck in rational drug discovery, particularly for complex diseases such as cancer and metabolic disorders, where subtle electronic effects and non-linear structure–activity relationships dominate ligand–target interactions. Classical machine learning and molecular simulation approaches have achieved notable success; however, they face fundamental limitations in efficiently representing high-dimensional quantum states governing intermolecular recognition.

This talk explores how quantum computing, in synergy with artificial intelligence, can be leveraged to enhance binding activity prediction at the molecular level. We present a hybrid quantum–classical framework that integrates quantum feature encoding of molecular descriptors, variational quantum circuits, and classical deep learning architectures to model drug–target interactions with improved expressivity and generalization. Case studies demonstrating how quantum-enhanced representations can capture subtle interaction patterns inaccessible to purely classical models.

We further outline the computational workflow, from molecular featurization and quantum state preparation to variational optimization and performance benchmarking against conventional cheminformatics pipelines. This work highlights the emerging role of quantum computing as a transformative technology for precision medicine, offering new paradigms for predicting binding activity and accelerating the discovery of next-generation therapeutics.

Fragment Molecular Orbital Study of the Photophysical Processes in Organic Semiconductor Materials

([1]*Institute for Quantum Life Science, National Institutes for Quantum Science and Technologies (QST)*) ○Takatoshi Fujita[1]

Keywords: Organic Photovoltaics; Exciton Dynamics; Charge Separation; Time-Resolved Spectroscopy

Organic electronic materials have attracted considerable interest due to their diverse functionalities in electronics and energy-related applications. They are composed of a disordered assembly of organic molecules or polymers. Accurate electronic structure calculations for such disordered molecular aggregates are still challenging. In addition, the elementary processes governing device properties, such as charge transport and charge photogeneration, are dynamical. Theoretical treatments of such dynamical processes require real-time simulations of electronic states in the presence of molecular vibrations and thermal fluctuations. To address these challenges, we have been developing multiscale simulation methods that combine ab initio electronic structure calculations with real-time quantum dynamics simulations. Specifically, to enable efficient and accurate electronic structure calculations, we have implemented the GW/Bethe-Salpeter equation (GW/BSE) method within the fragment molecular orbital (FMO) framework. Using the model excited-state Hamiltonian derived from the FMO method, the photophysical processes in realistic molecular aggregates can be simulated as the time evolutions of the excited-state wave functions.

As a representative application, we consider the charge-separation dynamics and pump-probe spectroscopy in the amorphous P3HT/PCBM blend (Fig. 1(a)). To simulate quantum dynamics and time-resolved spectroscopy, the model Hamiltonians for the single-excitation and double-excitation manifolds were derived using the FMO-GW/BSE method. After showing the energetics of the electron-hole separation (Fig. 1(b)) and the linear absorption spectrum (Fig. 1(c)), we investigate the quantum dynamics of exciton and charge carriers in comparison with the pump-probe transient absorption spectra. In particular, we introduce the pump-probe excited-state absorption (ESA) anisotropy as a spectroscopic signature of charge-carrier dynamics after exciton dissociation. We demonstrate that the charge-separation dynamics can be probed by the pump-probe ESA anisotropy dynamics following charge-transfer excitations.

Finally, we briefly present our recent efforts3 to obtain more reliable estimates of exciton dissociation time scales in donor/acceptor blends. To this end, we have introduced thermal or reorganization corrections into the wave packet dynamics method. Our results reveal that, in the presence of relatively high driving energy, higher-energy charge-transfer states are essential for the efficient exciton dissociation.

1) T. Fujita, Y. Noguchi, *J. Phys. Chem. A* **2021**, *125*, 10580. 2) T. Fujita, T. Hoshi, J. Phys. Chem. B **2023**, *127*, 7616. 3) T. Fujita, M. Nozaki, *Phys. Chem. Chem. Phys.* **2025**, *27*, 20765.

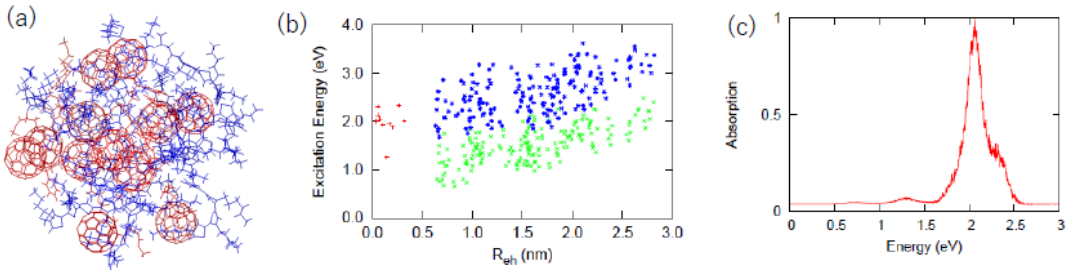

Figure.1(a)The atomistic structure of P3HT(blue)/PCBM(red) amorphous blend. (b) Electron-hole separation (nm) versus excitation energy and (c) absorption spectrum of the P3HT/PCBM blend.

Explicit-Solvent Molecular Dynamics Simulations: Reaction Dynamics and Thermodynamics

([1]*Graduate School of Urban Environmental Sciences, Tokyo Metropolitan University*)
○Tatsuhiro Murakami[1]
Keywords: Molecular Dynamics, Machine Learning Interatomic Potentials, Explicit solvent molecule, Message-passing neural network, MACE

Chemical reactions in condensed phases are governed not only by the intrinsic reactivity of the reactants but also by the surrounding solvent, which undergoes continual reorganization and can transiently stabilize reactive configurations through many-body interactions. Explicit-solvent molecular dynamics (MD) simulations are therefore essential when solvent reorientation, hydrogen-bond rearrangement, and entropic effects modulate reaction pathways, kinetics, and thermodynamic stability. In our previous work, explicit-solvent simulations at the semiempirical GFN2-xTB level demonstrated that dynamic solvation effects play a critical role in ionic dissociation dynamics and post-transition-state bifurcation behavior. [1–2] Nevertheless, semiempirical potentials often lack the quantitative accuracy required for reliable thermodynamic analysis and for evaluating energetics relevant to reactivity, whereas explicit-solvent simulations based on first-principles electronic-structure methods remain computationally prohibitive for extensive sampling, particularly for free-energy calculations.

In the present work, we develop a machine learning interatomic potential (MLIP) for target explicit-solvent systems using message-passing neural networks, focusing on the MACE (Message-Passing Atomic Cluster Expansion) model. The training set is generated from density functional theory (DFT) calculations on solvated cluster configurations sampled from preliminary NVT simulations performed with the GFN2-xTB potential. To enhance data efficiency and robustness, we pursue a transfer-learning strategy based on the pretrained MACE-OFF [3] model. As an initial step, MACE-OFF is benchmarked against DFT reference calculations for the target solvated configurations to evaluate its accuracy and transferability. Notably, MACE-OFF was trained on organic-molecule energies computed at the ωB97M-D3(BJ)/def2-TZVPPD level, and ORCA calculations at the same level are performed to provide consistent reference data for this validation.

Transfer learning via fine-tuning of the pretrained model is under development to obtain an MLIP that supports stable simulations across diverse solvent environments. An ML-driven explicit-solvent simulation workflow is being constructed with a primary focus on solvent-dependent thermodynamics under explicit solvation. Solvent-dependent free-energy differences between relevant molecular states are targeted for evaluation, and the preferentially stabilized state in each solvent is to be identified, thereby quantifying how

solvent environments reshape free-energy landscapes and control relative thermodynamic preferences. The scope emphasizes solvent-driven stabilization and free-energy changes, with mechanistic interpretation discussed in terms of solvent-structure fluctuations and reorganization patterns relevant to reactivity.

1) T. Murakami *et al*, *Molecules* **2025**, *30*, 442.
2) T. Murakami *et al.*, *ChemPhysChem* **2025**, *26*, e202500494.
3) D. P. Kovács, *et al., J. Am. Chem. Soc.,* **2025**, *147,* 17598.