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PART I ANNUAL REPORTS

1. Abstracts of Papers Published in Journals

MATHEMATICS

Construction of Non-prehomogeneous Polynomials with Local Functional Equations from Representations of Clifford Algebras

Fumihiro Sato* and Takeyoshi Kogiso (* Department of Mathematics, Rikkyo University)
Vestnik Tambou, **T. 16**, 1744-1750 (2011).

We give a new systematic construction of polynomials satisfying a functional equation, which are not relative invariants of prehomogeneous vector spaces. The construction depends on the pull back theorem of local functional equations.

A Classification of Some Prehomogeneous Vector Spaces Related with Hypergeometric Functions

T. Kimura*, T. Kogiso and M. Ouchi* (* Institute of Mathematics, University of Tsukuba)
Josai Mathematical Monograph, **5**, 89-111 (2012).

In this paper, we give the detailed proof of a classification of finite reductive prehomogeneous vector spaces of type $((Sp_{m_1} \times GL_{m_2} \times GL_1) \times GL_n, (\Lambda_1 \boxplus \Lambda_1 \boxplus \Lambda_1) \otimes \Lambda_1)$ ($m_1 \geq 2, n \geq 4$) under various restricted scalar multiplications, which are omitted in [KKMOT]. They are related with hypergeometric functions [O].

Prehomogeneous Vector Spaces and Their Regularity

T. Kimura*, T. Kogiso, Y. Kurosawa* and M. Ouchi* (* Institute of Mathematics, University of Tsukuba)
Josai Mathematical Monograph, **5**, 71-89 (2012).

In this paper, we gather the various known constructions of prehomogeneous vector spaces and give some new results. We consider everything over the complex number field \mathbb{C} .

Representations of Clifford Algebras and Local Functional Equations

F. Sato* and T. Kogiso (* Department of Mathematics, Rikkyo University)
RIMS Kokyuroku Bessatsu, **B36**, 53-66 (2012).

Let C_p (resp. C_q) be the Clifford algebra of a positive definite real quadratic form in p (resp. q) variables. For a representation ρ of $C_p \otimes C_q$, we can associate a homogeneous polynomial

P of degree 4 on the representation space of ρ having the property. The Fourier transform of the complex power $|P|^s$ coincides with $|P|^{-m/4-s}$ ($m =$ the degree of ρ) with an explicit gamma factor. According to the theory of prehomogeneous vector spaces, the basic relative invariant of an irreducible regular prehomogeneous vector space satisfies the property above. However the polynomials P are not necessarily relative invariants of any prehomogeneous vector spaces. The polynomials P are relative invariants of prehomogeneous vector spaces only for quite few exceptional cases. In this paper, we discuss the structure and the action of the group of linear transform actions that leave P invariant.

Fourier Transforms of Polynomials and Prehomogeneous Vector Spaces

T. Kogiso

Proceedings of the 7th International Conference on Nonlinear Analysis and Convex Analysis -I-, 241-254 (Bsan, Korea, 2011).

In this paper, we survey the fundamental theorem of prehomogeneous vector spaces which is related to a certain problem of Fourier transform of polynomials and give a recent result of this field.

On a Certain Class of Cuspidal Prehomogeneous Vector Spaces and Its Basic Relative Invariants

T. Kogiso and Y. Kurosawa* (* Institute of Mathematics, University of Tsukuba)

Josai Mathematical Monograph, **6**, 125-136 (2013).

In this paper, we give a certain class of cuspidal prehomogeneous vector spaces and determine explicitly two basic relative invariants of a cuspidal prehomogeneous vector space ($GL(4) \times GL(3) \times SL(2)$, $\Lambda_1^* \otimes 1 \otimes 1 + \Lambda_1 \otimes \Lambda_1^* \otimes \Lambda_1^*$, $M(1,4) \oplus M(4,3) \oplus M(4,3)$) which is a special case of the class. We consider everything over the complex number field \mathbb{C} .

Periodically Growing Solutions in a Class of Strongly Monotone Semiflows

Ken-Ichi Nakamura* and Toshiko Ogiwara (* Graduate School of Natural Science and Technology, Kanazawa University)

Networks and Heterogeneous Media, **7**, 881-891 (2012).

We study the behavior of unbounded global orbits in a class of strongly monotone semiflows and give a criterion for the existence of orbits with periodic growth. We also prove the uniqueness and asymptotic stability of such orbits. We apply our results to a certain class of nonlinear parabolic equations including a weakly anisotropic curvature flow in a two-dimensional annulus and show the convergence of the solutions to a periodically growing solution which grows up in infinite time changing its profile time-periodically.

Exact Construction of Liu Process

Kakuzo Iwamura and Masayuki Kageyama* (* The Institute of Statistical Mathematics, Tokyo)

Applied Mathematical Sciences, **6**, 2871-2880 (2012).

In this paper, we show how to fully mathematically create Liu process in credibility theory.

Existence Proof of Finitely Many Independent Fuzzy Vectors

Kakuzo Iwamura, Masayuki Kageyama*¹ and Shigeru Kitakubo*² (*1 The Institute of Statistical Mathematics, Tokyo, *2 Nippon Institute of Technology, Japan)

Pioneer Journal of Mathematics and Mathematical Sciences, **5**, 7-14 (2012).

This paper shows existence proof of finitely many independent fuzzy vectors.

A Sufficient and Necessary Condition of Uncertain Measure

Zixiong Peng* and Kakuzo Iwamura (* Tsinghua University, Beijing)

INFORMATION, **15**, 1381-1391 (2012).

Uncertainty theory is a branch of mathematics for modeling human uncertainty based on normality, duality, subadditivity, and product axioms. This paper gives a relation between set functions and uncertain measures, and proves a sufficient and necessary condition for uncertain measures. Finally, some examples are given.

Some Properties of Product Uncertain Measure

Zixiong Peng* and Kakuzo Iwamura (* Tsinghua University, Beijing)

Journal of Uncertain Systems, **6**, 263-269 (2012).

Uncertainty theory is a branch of mathematics for modeling human uncertainty. The first fundamental concept in uncertainty theory is uncertain measure, which is defined by normality axiom, duality axiom and subadditivity axiom. The second fundamental concept is the product uncertain measure, which is defined by product axiom. This paper shows that the product uncertain measure is indeed an uncertain measure, which also means that the product axiom is consistent with other axioms in uncertainty theory.

PHYSICS

Measurements and Phase-Shift Analysis of the Differential Cross Sections for the Elastic Scattering in C^{2+} - He System at $E_{cm} = 2.8$ eV

Yoh Itoh

J. Phys. Soc. Jpn. **81**, 065002 (2012).

http://libir.josai.ac.jp/il4/meta_pub/G0000002repository_JOS-JPSJ.81.065002

Using a crossed-beam apparatus, we determined the relative differential cross sections for the elastic scattering in C^{2+} - He system at $E_{cm} = 2.8$ eV. The measured cross sections were compared with the calculated ones based on the interaction potentials obtained by *ab initio* calculations. The analysis revealed that the measured structure in the differential cross sections is due to the rainbow scattering; however, the well depth of the *ab initio* potentials reported was found to be not deep enough to reproduce the rainbow-angle measured.

CHEMISTRY

A Molecular Orbital Study of the Dipole Moment of HF, LiH, and HeH⁺

Hiroyuki Teramae, Shin-ichi Nagaoka,^{*1} and Umpei Nagashima^{*2} (*1 Ehime University, *2 National Institute of Advanced Industrial Science and Technology)

Chem. Lett., **41**, 1642-1643 (2012)

The threshold bond distances of electron transfer in the typical heteronuclear diatomic molecules, HF, LiH, and HeH⁺ have been studied in conjunction with the dipole moments by using *ab initio* molecular orbital method. The electron transfer begins at 3Å for HF, 6Å for LiH, and 4Å for HeH⁺, and the dipole moments have their maxima at 1.2Å for HF, 2.4Å for LiH, and 0.8Å after the electrostatic correction for HeH⁺.

Theoretical Study on Ground and Excited States of 3,5-diacetyl-1,4-dihydrolutidine

Hiroyuki Teramae, Yasuko Y. Maruo, Jiro Nakamura

Intern J. Chem. Model. **4**, 49-55 (2012).

The ground and excited state of 3,5-diacetyl-1,4-dihydrolutidine (DL1) are calculated with the *ab initio* molecular orbital method at HF/3-21G, CIS/3-21G, B3LYP/6-31G**, and TD B3LYP/6-31G** levels. As a model for the DL1 in aqueous solution and porous glass, the geometries of complexes of DL1 and water, and that of DL1 and H₂Si=O are also optimized at B3LYP/6-31G** and HF/6-31G** levels. The excited states of these complexes are also calculated at TD B3LYP/6-31G** and CIS/6-31G** levels. The excited states of these two com-

plexes are found to be totally different from each other. The LUMO of DL1-H₂Si=O complex is consisted with the LUMO of H₂Si=O, whereas the LUMO of DL1-water complex is consisted with the LUMO of DL1. This fact suggests that the electronic structure of the excited state of the lutidine compounds (DL1) would be different in the aqueous solution and in the porous glass.

窒素分子 N₂ の最高被占軌道 HOMO は σ 型か π 型か？

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J. Comp. Chem. Japan, **11**, 89-92 (2012)

窒素分子 N₂ は 3 重結合を持つ等核 2 原子分子として多くの教科書で紹介されているが, その電子状態に関する記述は最高占有軌道を σ 型とするものと π 型とするものがあり, まだ定まっていない. 本論文では核間距離に関する分子軌道エネルギーの変化を示し, 平衡核間距離付近の窒素分子 N₂ 最高占有軌道が π 型であることを示す. 用いた計算方法は RHF/6-311G** である. 平衡核間距離 (1.0703 Å) 近傍の最高占有軌道は π 型であるが, 核間距離が 1.045 Å より短くなると σ 型となる.

The Dielectric Constant Dependence of Absorption Intensities and Wavenumbers of the Fundamental and Overtone Transitions of Stretching Vibration of the Hydrogen Fluoride Studied by Quantum Chemistry Calculations

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J. Mol. Structure. **1018**, 102-106 (2012).

Vibrational potentials and dipole moment functions of HF molecule in solutions have been calculated as a function of dielectric constant by using the self-consistent reaction field (SCRf)/isodensity surface polarized continuum model (IPCM) calculation. We have selected HF molecule as the simplest polar molecule. The wavenumbers and absorption intensities of the fundamental and the first, second and third overtones of H-F stretching mode have been calculated as a function of dielectric constant. The SCRf/IPCM model calculations have revealed that the vibrational potential and dipole moment function of HF molecule vary continuously with a change in the dielectric constant of the solvent. The calculations were carried out at B3LYP/6-311++G(3df,3pd) and CCSD/aug-cc-pVQZ levels. It has also been found that the absorption intensities of the fundamental increase with the increase of the dielectric constant smoothly but those of the first, second and third overtones do not increase continuously. Moreover, the B3LYP and CCSD levels yielded significantly different results in the dependence of absorption intensities on the dielectric constant.

Design of velocity map imaging spectrometer equipped with a mass gate discriminating particular photofragments

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ISRN Phys. Chem., **2012**, 959074 (9 pages) (2012)

A photoionization spectrometer for velocity map imaging has been developed for measuring the scattering distribution of fragment ions from polyatomic molecules. The spectrometer contains a mass gate and an ion reflector which are able to discriminate ions with a particular mass-to-charge ratio m/z . The basic functions and feasibility of these devices were tested experimentally and theoretically. First, the photoions from Kr and C_{60} were extracted into a time-of-flight (TOF) mass spectrometer by a transient or continuous electrostatic field. When the pulse application on the mass gate was tuned to the arrival timing of ions with a specific m/z , the peak of the selected ions alone was present on a TOF spectrum. Second, compatibility between velocity map imaging and ion discrimination was investigated by the computer simulations of the ion trajectories of photofragments from C_{60} . A pulsed voltage was applied to the mass gate synchronously with the arrival timing of C_{58}^+ ions. The initial three-dimensional velocity distribution of C_{58}^+ was projected onto the image plane with an energy resolution better than 10 meV. The C_{58}^+ image was free from the contamination of other ions such as C_{60}^+ and C_{56}^+ .

Nanosecond simulations of the dynamics of C_{60} excited by intense nearinfrared laser pulses: Impulsive Raman excitation, rearrangement, and fragmentation

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J. Chem. Phys., **136**, 164304 (12 pages) (2012)

Impulsive Raman excitation of C_{60} by single or double pulses of near-infrared wavelength $\lambda = 1800$ nm was investigated by using a time-dependent adiabatic state approach combined with the density functional theory method. We confirmed that the vibrational energy stored in a Raman active mode of C_{60} is maximized when $T_p \sim T_{\text{vib}}/2$ in the case of a single pulse, where T_p is the pulse length and T_{vib} is the vibrational period of the mode. In the case of a double pulse, mode selective excitation can be achieved by adjusting the pulse interval τ . The energy of a Raman active mode is maximized if τ is chosen to equal an integer multiple of T_{vib} and it is minimized if τ is equal to a half-integer multiple of T_{vib} . We also investigated the subsequent picosecond or nanosecond dynamics of Stone-Wales rearrangement (SWR) and fragmentation by using the density-functional based tight-binding semiempirical method. We present how SWRs are caused by the flow of vibrational kinetic energy on the carbon bond network of C_{60} . In the case where the $h_g(1)$ prolate-oblate mode is initially excited, the

number of SWRs before fragmentation is larger than in the case of $a_g(1)$ mode excitation for the same excess vibrational energy. Fragmentation by C_2 ejection $C_{60} \rightarrow C_{58} + C_2$ is found to occur from strained, fused pentagon/pentagon defects produced by a preceding SWR, which confirms the earliest mechanistic speculations of Smalley *et al.* [J. Chem. Phys. **88**, 220 (1988)]. The fragmentation rate of C_2 ejection in the case of $h_g(1)$ mode excitation does not follow a statistical description as employed for instance in the Rice-Ramsperger-Kassel (RRK) theory, whereas the rate for $a_g(1)$ mode excitation does follow the prediction by RRK. We also found for the $h_g(1)$ mode excitation that the nonstatistical nature affects the distribution of barycentric velocities of fragments C_{58} and C_2 . This result suggests that it is possible to control rearrangement and subsequent bond breaking in a “nonstatistical” way by initial selective mode excitation.

Multiplex-PCR 法によるフクロアミ属 2 種の簡易識別法

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DNA 多型, **20**, 114-118 (2012)

ナミフクロアミとシキシマフクロアミは、およそ 1 cm 弱の大きさで、共に海岸から近く比較的水深の浅い砂の中に生息する潜砂性のアミである。両種が同所的に生息する海域で両種の生態を調べるためには、種の同定が正確に行われる必要がある。しかし、両種の形態学的な識別は難しい。そのため、分子マーカーを用いた簡便な識別法を開発した。本研究では、ある種に特異的なプライマーを用いて他の種との差異を検出する種特異的プライマーを用いた Multiplex-PCR 法を採用した。ナミフクロアミとシキシマフクロアミ各 4 個体のミトコンドリア DNA CO I 遺伝子領域を PCR 法により増幅し、塩基配列を決定した。両種間の変異の大きなサイトを選定し、L 鎖側にナミフクロアミ特異的プライマーとシキシマフクロアミ特異的プライマーの 2 つの種特異的プライマーを作製した。H 鎖側のユニバーサルプライマーを加えた Multiplex-PCR を行った結果、ナミフクロアミでは約 490 塩基の、シキシマフクロアミでは約 330 塩基の PCR 産物が得られ、サイズの違いから 2 種を判別することができた。この識別法は 1 回の PCR と電気泳動で結果が得られるという迅速さも利点であるといえる。

カジカ類 4 種のミトコンドリアゲノム全塩基配列の比較

石黒直哉, 長谷川喬之^{*1} (*1 福井工大工)

DNA 多型, **20**, 119-126 (2012)

日本列島を含む東ユーラシア地域に生息するカジカ類は、種が降河回遊性や両側回遊性、また河川性などの多様な生活史を示すために、それらの種分化に関心が集まっている。よって、カジカ属 3 種 (カマキリ, エゾハナカジカ, カジカ中卵型) の mtDNA の全塩基配列を決定し、既知のウツセミカジカを含めた 4 種間で mtDNA の比較を行った。決定できた 3 種の全塩基数は、16,506 ~ 16,566 bp であり、遺伝子の配置は典型的な脊椎動物と同様であった。しかしながら、50 bp 以下の小さい非コード領域が 2 ヶ所見つかった。一つ (tRNA^{Asp} と CO II の間) は、エゾ

ハナカジカ, カジカ中卵型, ウツセミカジカの3種に, もう一つ (tRNA^{Thr} と tRNA^{Pro} の間) は, カジカ中卵型, ウツセミカジカの2種にみられた。Yokoyama and Goto (2005) の系統仮説から, まずカマキリと他のカジカ属との分岐後に, カマキリ以外のカジカ属のクレードで前者の非コード領域が挿入され, 次に, エゾハナカジカやハナカジカ, カンキョウカジカのグループとウツセミカジカやカジカ種群のクレードとの分岐後に, ウツセミカジカとカジカ種群のクレードで後者のそれが挿入されたと考えられる。

Photofabrication of fullerene-shelled quantum dots supramolecular nanoparticles for solar energy harvesting

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ACS Nano, **6**, 1601-1608 (2012)

Quantum dots-based electron donor-acceptor systems play a rising role in the design of renewable and carbon-free energy harvesting technologies. In this article, we discuss the photofabrication of fullerene-shelled quantum dots supramolecular nanoparticles, in which the fullerene shell acts as not only a well-defined electron acceptor but also a robust protecting layer against the photocorrosion of the quantum dot core. We evaluate the ensemble and single-molecule electron transfer from the core to the shell in the nanoparticles and the photocurrent response of a photoelectrochemical cell constructed using the nanoparticles. The supramolecular nanoparticle has been prepared by the covalent tethering of a fullerene-thiol monolayer to the quantum dot followed by the photochemical reactions of free fullerene-thiol to the tethered monolayer. The nanoparticles are characterized using scanning electron microscopy, atomic force microscopy, and X-ray photoelectron spectroscopy. Correlated single-photon emission and the two-state ON-OFF photoluminescence show that single quantum dots are included in the supramolecular nanoparticles. The fullerene-shells suppress the blinking of single quantum dots by acting as well-defined electron traps, without allowing the transfer of Auger electrons to unknown traps. Electron transfer from the quantum dot-core to the fullerene-shell is apparent from the short ON and OFF durations in the photoluminescence intensity trajectories of single quantum dots, quenching of the photoluminescence intensity and lifetime of quantum dots at the ensemble level, and the characteristic transient absorption band of the anion radical of fullerene. We next construct a photoelectrochemical cell using the supramolecular nanoparticles, and the transferred electron is externally driven in the cell to generate $\sim 400 \mu\text{A}/\text{cm}^2$ photocurrent. Electron transfer from the highly stable quantum dots to the protecting fullerene-shells places the supramolecular nanoparticles among the most promising antenna systems for the construction of cost-effective and stable next generation solar energy harvesting systems.

FRET from quantum dots to photodecompose undesired acceptors and report the condensation and decondensation of plasmid DNA

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ACS Nano, **6**, 3776–3788 (2012)

Protection of genes against enzymatic degradation and overcoming of cellular barriers are critical for efficient gene delivery. The effectiveness of gene delivery by nonviral vectors depends mostly on the extent of DNA packaging or condensation. We show that Förster resonance energy transfer (FRET)-mediated photodecomposition of undesired acceptors in doubly labeled plasmid DNA (pDNA) and FRET recovery after acceptor photodecomposition (FRET-RAP) are effective methods for the detection of DNA condensation and decondensation. Our hypothesis is that undesired acceptors within the Förster distance of highly-photostable donors in precondensed DNA can be selectively photodecomposed by FRET. We investigate this hypothesis by the random labeling of pcDNA3.1-GL3 and pUC18DNA with quantum dots (QDs) as the energy donor and AlexaFluor594 or Cy5 as the acceptor. At first, the random labeling generates efficient FRET, also called intrinsic FRET, in precondensed DNA, which prevents us from decoding any changes in the FRET efficiency during DNA condensation. Next, we suppressed the intrinsic FRET by the FRET-mediated photodecomposition of acceptors within the Förster distance of QDs. Conversely, many acceptors kept intact beyond the Förster distance provide us with high FRET efficiency during the condensation of pDNA using protamine. Further, the FRET efficiency is significantly decreased during the decondensation of DNA using heparan sulfate and glutathione. The random labeling of DNA using excess acceptors around photostable donors followed by the FRET-mediated photodecomposition of undesired acceptors can be a promising method for not only the sensitive detection of DNA condensation by FRET but also the customization of biomolecular sensors.

Inhibition Assay of Yeast Cell Walls by Plasmon Resonance Rayleigh Scattering and Surface-enhanced Raman Scattering Imaging

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Langmuir, **28**, 8952–8958 (2012).

We report on plasmon resonance Rayleigh scattering (PRRS) and surface enhanced Raman scattering (SERS) imaging for inhibition assay of yeast cell walls. This assay reveals that the proteins having alkali sensitive linkage bound to β 1,3 glucan frameworks in cell walls are involved in SERS activity. The result is further confirmed by comparison of genetically modified cells and wild type cells. Finally, we find that PRRS and SERS spots do not appear

on cell walls when daughter cells are enough smaller than parent ones, but appear when size of daughter cells are comparable to parent cells. This finding indicates the relationship between expression of the proteins that generate SERS spots and cell division. These results demonstrate that PRRS and SERS imaging can be a convenient and sensitive method for analysis of cell walls.

Quantitative evaluation of blinking in surface enhanced resonance Raman scattering and fluorescence by electromagnetic mechanism

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J. Chem. Phys., **136**, 024703 (2012).

We analyze blinking in surface enhanced resonance Raman scattering (SERRS) and surface enhanced fluorescence (SEF) of rhodamine 6G molecules as intensity and spectral instability by electromagnetic (EM) mechanism. We find that irradiation of intense NIR laser pulses induces blinking in SERRS and SEF. Thanks to the finding, we systematically analyze SERRS and SEF from stable to unstable using single Ag nanoparticle (NP) dimers. The analysis reveals two physical insights into blinking as follows. (1) The intensity instability is inversely proportional to the enhancement factors of decay rate of molecules. The estimation using the proportionality suggests that separation of the molecules from Ag NP surfaces is several angstroms. (2) The spectral instability is induced by blue shifts in EM enhancement factors, which have spectral shapes similar to the plasmon resonance. This analysis provides us with a quantitative picture for intensity and spectral instability in SERRS and SEF within the framework of EM mechanism.

How environmental solution conditions determine the compaction velocity of single DNA molecules

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Nucleic Acids Res., **40**, 284–289 (2012).

Understanding the mechanism of DNA compaction is becoming increasingly important for gene therapy and nanotechnology DNA applications. The kinetics of the compaction velocity of single DNA molecules was studied using two non-protein condensation systems, poly (ethylene glycol) (PEG) with Mg^{2+} for the polymer-salt-induced condensation system and spermine for the polyamine condensation system. The compaction velocities of single tandem λ DNA molecules were measured at various PEG and spermine concentrations by video fluorescence microscopy. Single DNA molecules were observed using a molecular stretching technique in the microfluidic flow. The results show that the compaction velocity of a single DNA molecule

was proportional to the PEG or spermine concentration to the power of a half. Theoretical considerations indicate that the compaction velocity is related to differences in the free energy of a single DNA molecule between the random coil and compacted states. In the compaction kinetics with PEG acceleration of the compaction velocity occurred above the overlap concentration while considerable deceleration occurred during the coexistence state of the random coil and the compacted conformation. This study demonstrates the control factors of DNA compaction kinetics and contributes toward the understanding of the compaction mechanisms of non-protein DNA interactions as well as DNA-protein interactions *in vivo*.

Studies on the Interaction of Pulsed Lasers with Plasmonic Gold Nanoparticles toward Light Manipulation, Heat Management, and Nanofabrication

Daniel Werner^{*1}, Shuichi Hashimoto^{*1}, Takayuki Uwada (*1 Department of Ecosystem Engineering, The University of Tokushima)

J. Photochem. Photobiol. C, **13**, 28-54 (2012)

This review describes the fundamental aspects of laser-gold nanoparticle (Au NP) interaction that leads to nanoscale energy deposition to the surroundings through light amplification and heat generation. Besides the importance of the primary process in physics and chemistry, application of the light-NP interaction has attracted significant interest from various areas ranging from analytical chemistry to material chemistry and biomedicine. Here we consider both mechanistic and application aspects. Our attention is focused on pulsed-laser-induced fast processes that revealed the heating-cooling dynamics of electrons, lattice (particle), and particle's environment. On the application side, we focus on material fabrication and processing that beat diffraction-limited resolution. Together, we will shed a light on the essence of research activities carried out in the past 10 years. In addition to an abundance of latest information obtained from currently available literature, this review includes figures obtained by our own calculations to provide readers with a better understanding of the basics of the optical properties and energy and heat-transfer processes of Au NPs, which are not familiar to photochemists.

Glycine Crystallization in Solution by CW Laser-Induced Microbubble on Gold Thin Film Surface

Takayuki Uwada, Sho Fujii^{*1}, Teruki Sugiyama^{*2}, Anwar Usman^{*3}, Katsuhiko Kanaizuka^{*1}, Masa-aki Haga^{*1}, Atsushi Miura^{*3}, Hiroshi Masuhara^{*3} (*1 Department of Applied Chemistry, Faculty of Science and Engineering, Chuo University, *2 Instrument Technology Research Center, National Applied Research Laboratories, Taiwan, *3 Department of Applied Chemistry and Institute of Molecular Science, National Chia Tung University, Taiwan)

ACS Appl. Mat. Interfaces, **4**, 1158-1163 (2012)

We have developed a novel laser-induced crystallization method utilizing local heat-

induced bubble/water interface. Continuous laser beam of 1064 nm is focused on a gold nanoparticles thin film surface covered with glycine supersaturated aqueous solution. Light absorption of the film due to localized plasmon resonance caused local heating at the focal position and produced a single thermal vapor microbubble, which generated thermal gradient followed by convection flow around the bubble and eventually induced glycine crystallization and growth. The crystallization mechanism is discussed by considering gathering and accumulating molecules around the bubble/water interface assisted by convection flow and temperature jump.

Laser Trapping-Induced Reconfiguration of Individual smectic Liquid Crystal Micro-droplet Showing Size-dependent Dynamics

Anwar Usman^{*1}, Wei-Yi Chiang^{*1}, Takayuki Uwada, Hiroshi Masuhara^{*1} (*1 Department of Applied Chemistry and Institute of Molecular Science, National Chiao Tung University, Taiwan)
Proc. SPIE, **8274**, 82740L1-8 (2012)

We present laser trapping behavior of individual smectic 4'-n-pentyl-4-cyanobiphenyl liquid crystalline micro-droplet dispersed in heavy water; in particular, laser trapping-induced molecular reconfiguration of the optically trapped droplet when the laser trapping power is above a definite threshold. The reconfiguration undergoes throughout the inside of the droplets even though their size is larger than the focal spot, and the threshold laser power depends on the droplet size. We propose that the reconfiguration mechanism involves optical reorientation at the focal volume competing with the droplet-liquid interfacial anchoring effect, leading to symmetry breaking throughout the inside of the optically confined droplet. With this mechanism, we qualitatively described the existence of the threshold power and the dependence of the threshold upon the droplet size.

Novel rearrangements in the reactions directed toward preparation of spiro-*N,N*-ketals: Reactions of naphthalene-1,8-diamine with ninhydrin and isatin

Motoko Akita, Hideyuki Seto, Reiko Aoyama, Junko Kimura, and Keiji Kobayashi
Molecules, **17**, 13879-13890 (2012).

Spiro-*N,N*-ketal **5** consisting of a phthaloperine heterocyclic ring and a naphtha [1,8-ef] [1,4] diazepin ring was obtained along with spiro-*N,N*-ketal **2** via 2,2-condensation from the reaction of ninhydrin with naphthalene-1,8-diamine. Their molecular structures were elucidated by X-ray crystal structural analysis. Aside from these spiro compounds, the diazapleidiene compound **3** formed by 1,2-condensation and the 1,4-isoquinolinedione compound **4** arising from ring expansion were isolated. When isatin was reacted with naphthalene-1,8-diamine, spiro-*N,N*-ketal **6** and the two 1*H*-perimidine-based compounds **7** and **8** were isolated. **8** was revealed to be in a fast dynamic prototropic tautomerization in solution. Plausible mechanisms of the formation of the products are proposed.

Photoluminescence Properties, Molecular Structures, and Theoretical Study of Heteroleptic Silver(I) Complexes Containing Diphosphine Ligands

Satoshi Igawa, Masashi Hashimoto, Isao Kawata, Mikio Hoshino, and Masahisa Osawa
Inorg. Chem., **51**, 5805-5813 (2012)

The homoleptic complex $[\text{Ag}(\text{L})_2]\text{PF}_6$ (1) and heteroleptic complexes $[\text{Ag}(\text{L})(\text{LMe})]\text{BF}_4$ (2) and $[\text{Ag}(\text{L})-(\text{LEt})]\text{BF}_4$ (3) [L = 1,2-bis(diphenylphosphino)benzene, LMe = 1,2-bis[bis(2-methylphenyl)phosphino]benzene, and LEt = 1,2-bis[bis(2-ethylphenyl)phosphino]benzene] were synthesized and characterized. X-ray crystallography demonstrated that 1-3 possess tetrahedral structures. Photophysical studies and time-dependent density functional theory calculations of 1-3 revealed that alkyl substituents at the ortho positions of peripheral phenyl groups in the diphosphine ligands have a significant influence on the energy and intensity of phosphorescence of the complex in solution at room temperature. The results can be interpreted in terms of the geometric preferences of each complex in the ground and excited states. The homoleptic complex 1 exhibits weak orange phosphorescence in solution arising from its flat structure in the triplet state, while heteroleptic complexes 2 and 3 show strong green phosphorescence from triplet states with tetrahedral structure. Larger interligand steric interactions in 2 and 3 caused by their bulkier ligands probably inhibit geometric relaxation within the excited-state lifetimes, leading to higher energy phosphorescence than that observed for 1. NMR experiments revealed that 2 and 3 in solution possess structures that are much more immobilized than that of 1; fluxional motion is completely suppressed in 2 and 3. Accordingly, conformational changes of 2 and 3 are expected to be suppressed by the alkyl substituents not only in the ground state but also in excited states. Consequently, nonradiative decay of the excited states of 2 and 3 occurs less efficiently than in 1. As a result, the quantum yields of phosphorescence for 2 and 3 are 6 times larger than that for the homoleptic complex 1.

2. Books, Reviews and Other Printings

MATHEMATICS

関数等式と表現論

小木曾岳義

数理科学 2013 年 1 月号 特集：「表現論の世界」, サイエンス社, 34-39 (2013).

CHEMISTRY

Non-Born-Oppenheimer analysis for the rotational and vibrational-rotational spectra of diatomic molecules

Hiroichi Uehara

Recent Res. Devel. Chem. Phys., Vol. 6, Transworld Research Network, Kerala, pp. 79-110 (2012).

Simulation of nuclear dynamics of C_{60} : from vibrational excitation by near-IR femtosecond laser pulses to subsequent nanosecond rearrangement and fragmentation

Naoyuki Niitsu^{*1}, Miyu Kikuchi^{*1}, Hayato Ikeda^{*1}, Kaoru Yamazaki^{*1}, Manabu Kanno^{*1}, Hirohiko Kono^{*1}, Koichiro Mitsuke, Mikito Toda^{*2}, Katsunori Nakai^{*3}, and Stephan Irle^{*4} (*1 Tohoku University, *2 Nara Women's University, *3 The University of Tokyo, *4 Nagoya University)

Quantum Systems in Chemistry and Physics: Progress in Methods and Applications, Eds. K. Nishikawa, J. Maruani, E. J. Brändas, G. Delgado-Barrio, and P. Piecuch; Springer, pp. 149-177 (2012)

Simulation of nuclear dynamics of C_{60} : from vibrational excitation by near-IR femtosecond laser pulses to subsequent nanosecond rearrangement and fragmentation

Naoyuki Niitsu^{*1}, Miyu Kikuchi^{*1}, Hayato Ikeda^{*1}, Kaoru Yamazaki^{*1}, Manabu Kanno^{*1}, Hirohiko Kono^{*1}, Koichiro Mitsuke, Mikito Toda^{*2}, Katsunori Nakai^{*3}, and Stephan Irle^{*4} (*1 Tohoku University, *2 Nara Women's University, *3 The University of Tokyo, *4 Nagoya University)

Quantum Systems in Chemistry and Physics: Progress in Methods and Applications, Eds. K. Nishikawa, J. Maruani, E. J. Brändas, G. Delgado-Barrio, and P. Piecuch; Springer, pp. 149-177 (2012)

“赤魚”のDNA鑑定

石黒直哉, 平林裕一郎*¹ (*1 福井工大工)
福井工業大学研究紀要, **42**, CD-ROM (2012)

Non-blinking semiconductor nanocrystals

石川 満

Part I, 4章, 論文にみる最重要概念と革新実験データ, pp.20-23.
CSJ Current Review 「ここまで進んだバイオセンシング・イメージング——1分子から細胞, 脳まで」日本化学会編, 化学同人, 2012.

演習でクリア「フレッシュマン有機化学」

小林啓二

裳華房, 1-204 ページ, 2012年

EARTH SCIENCE

地学現象の再現実験——洗濯糊 (Polyvinyl alcohol: PVA) スライムを用いた粘弾性流体の再現——

谷口英嗣, 町田嗣樹*¹, 齋藤洋輔*² (*1 早稲田大学創造理工学部環境資源工学科, *2 茗溪学園高等学校)
城西大学研究年報 (自然科学編), **35**, 13-22 (2012)

PHYSICAL EDUCATION

バレーボール選手の競技能力判定法に関する研究

明石正和, 川之上豊*¹, 横矢勇一*², 田中信雄*³ (*1 大妻女子大学, *2 大東文化大学(非), *3 京都産業大学文化学部)
城西大学研究年報 (自然科学編), **34**, 47-59 (2011)

バレーボール選手の競技能力判定法に関する研究 第2報 ——バレーボール指数について——

田中信雄*¹, 村上博巳*¹, 川之上豊*², 横矢勇一*³, 明石正和 (*1 京都産業大学文化学部, *2 大妻女子大学, *3 大東文化大学(非))
城西大学研究年報 (自然科学編), **35**, 23-40 (2012)

3. Oral Presentations

MATHEMATICS

Fourier Transforms of Polynomials and Prehomogeneous Vector Spaces

Takeyoshi Kogiso

Nonlinear Analysis and Convex Analysis International Conference (Pusan Korea), 2011 年 8 月

Clifford 代数の表現から得られる非概均質的局所関数等式について

小木曾岳義

表現論ワークショップ 2011 (鳥取), 2011 年 12 月

2 次写像についてのある考察

小木曾岳義

つくば国際会議場研究集会「概均質ベクトル空間」(つくば), 2012 年 1 月

Clifford 代数の表現から得られる局所関数等式について

小木曾岳義

日本数学会関数解析分科会特別講演 (東京), 2012 年 3 月

局所関数等式を満たす多項式のペアについて

小木曾岳義

筑波大学数学系特別セミナー (つくば), 2012 年 6 月

Clifford 代数の表現から得られる局所関数等式

小木曾岳義

近畿大学理工学部数学科講演会 (近畿大学), 2012 年 7 月

Quadratic Maps to PV's and Local Functional Equations

Takeyoshi Kogiso

Representations of algebraic groups and relate topics (JMM-workshop, Tokyo), 2012 年 9 月

Quadratic Maps to PV's and Local Functional Equations

Takeyoshi Kogiso

Kyoto Conference on Automorphicforms (Kyoto), 2012 年 10 月

PV の裏返し変換についての一考察

小木曾岳義

表現論ワークショップ (鳥取), 2012 年 12 月

Representations of Clifford Algebras and Local Functional Equations

小木曾岳義

九州大学大学院数理学府表現論セミナー (九州大学), 2013 年 3 月

Convergence Results in Order-preserving Dynamical Systems and Applications to a Molecular Motor System

Toshiko Ogiwara

Nonlinear Partial Differential Equations, Dynamic Systems and Their Applications (京都大学), 2012 年 9 月

順序保存力学系と生物分子モーターモデルへの応用

荻原俊子

京都駅前セミナー (京都), 2012 年 10 月

PHYSICS

C^{3+} - Ne 衝突における一電子移行過程の微分断面積測定

伊藤 陽

日本物理学会 2012 年秋季大会 (横浜国立大学), 2012 年 3 月, 講演概要集 第 2 分冊
21aAJ-7

CHEMISTRY

エタノールアミン・ジエタノールアミンの構造に関する分子軌道計算

寺前裕之, 丸尾容子*¹ (*1 NTT 環境エネルギー研)

第 15 回理論化学討論会 (仙台), 2011 年 6 月, 講演要旨集 2P02

ルチジン誘導体生成の反応機構に関する理論的研究

石川諒, 寺前裕之, 丸尾容子^{*1} (*1 NTT 環境エネルギー研)
日本コンピュータ化学会 2012 年春季年会 (東京), 2012 年 5 月, 講演要旨集 1P16

エタノールアミン・ジエタノールアミンの構造に関する理論的研究

寺前裕之, 丸尾容子^{*1} (*1 NTT 環境エネルギー研)
日本コンピュータ化学会 2012 年春季年会 (東京), 2012 年 5 月, 講演要旨集 1P20

アセチルアセトン法によるルチジン誘導体の生成反応に関する理論的研究

寺前裕之, 丸尾容子^{*1} (*1 NTT 環境エネルギー研)
分子科学討論会 2012 (東京), 2012 年 9 月, 講演要旨集 3P116

分子軌道法による HF, LiH, HeH⁺ の双極子モーメント

寺前裕之, 長岡伸一^{*1}, 長嶋雲兵^{*2} (*1 愛媛大院理, *2 産総研)
日本コンピュータ化学会 2012 年秋季年会 (山形), 2012 年 10 月, 講演要旨集 1P02

ルチジン誘導体生成の反応機構に関する理論的研究 (2)

石川諒, 寺前裕之, 丸尾容子^{*1} (*1 NTT 環境エネルギー研)
日本コンピュータ化学会 2012 年秋季年会 (山形), 2012 年 10 月, 講演要旨集 2P05

エタノールアミンの構造に関する理論的研究

小藺貴幸, 寺前裕之, 丸尾容子^{*1} (*1 NTT 環境エネルギー研)
日本コンピュータ化学会 2012 年秋季年会 (山形), 2012 年 10 月, 講演要旨集 2P06

アセチルアセトン法によるルチジン誘導体の生成反応に関する理論的研究

寺前裕之, 丸尾容子^{*1} (*1 NTT 環境エネルギー研)
第 35 回情報化学討論会 (広島), 2012 年 10 月, 講演要旨集 P13

プロトン化水クラスターの安定構造の網羅的探索

赤瀬 大^{*1}, 相田美砂子^{*1}, 寺前裕之 (*1 広大院理)
第 35 回情報化学討論会 (広島), 2012 年 10 月, 講演要旨集 P14

Theoretical study on the reaction mechanism of formation of FLUORAL-P and lutidine derivatives

Hiroyuki Teramae, Yasuko Y. Maruo^{*1} (*1 *NTT Energy & Environmental Laboratories*)
ACS National Meeting 2012 Spring (San Diego), March 2012, COMP316

Theoretical study on the reaction mechanism of formation of lutidine derivatives

Hiroyuki Teramae, Yasuko Y. Maruo^{*1} (*1 *NTT Energy & Environmental Laboratories*)
ISOME2012 (Tokyo), June 2012, O7-3

Theoretical study on the structures of ethanolamine and its CO₂ complexes using the Hamiltonian algorithm

Hiroyuki Teramae, Yasuko Y. Maruo^{*1} (*1 *NTT Energy & Environmental Laboratories*)
ICQC2012 (Boulder), June 2012, III-26

Ab initio study on the reaction mechanism of formation of lutidine derivatives

Hiroyuki Teramae, Yasuko Y. Maruo^{*1} (*1 *NTT Energy & Environmental Laboratories*)
TACC-2012 (Pavia), September 2012.

二重試料高分解能赤外発光分光による GaF の振動回転スペクトルの精密な測定

勝家俊介, 角田典雅, 堀合公威, 上原博通
第6回分子科学討論会 (東京), 2012年9月, 3P008

二重試料高分解能赤外発光分光による AlH の振動回転スペクトルの精密な測定

矢部辰翔, 坂本幸博, 堀合公威, 上原博通
第6回分子科学討論会 (東京), 2012年9月, 3P009

ナノ孔ガラスを用いた気相トルエン濃度の近赤外分光測定

加藤靖子, 紺野東一, 尾崎 裕, 内山政弘^{*1}, 長澤 浩^{*2} (*1 国立環境研究所, *2 ナノ・サポート(株))
日本化学会第92春季年会 (日吉), 2012年3月

Kr-C¹⁶O¹⁸O 錯体の赤外ダイオードレーザー分光

渋谷 健, 女屋 敬, 紺野東一, 尾崎 裕
第6回分子科学討論会 (東京), 2012年9月

van der Waals 錯体 希ガス — シクロブタンの構造の量子化学計算

宮川 肅, 紺野東一, 尾崎 裕

第6回分子科学討論会 (東京), 2012年9月

Morphology, catalytic activities, and electronic structures of the nanosystems constituting dye-sensitized solar cells

Koichiro Mitsuke

The 27th Philippine Chemistry Congress (Manila), 2012年4月 (Invited)

Measurement of kinetic energies of fragments produced by the photodissociation of C₇₀ using velocity map imagingHideki Katayanagi^{*1} and Koichiro Mitsuke (*1 Institute for Molecular Science)

JST International Symposium on Multi-scale Simulation of Condensed-phase Reaction Systems (MSCRS2012) (Nagoya), 2012年5月

Photodissociation dynamics of C₇₀ studied by velocity map imaging with an improved mass resolutionHideki Katayanagi^{*1} and Koichiro Mitsuke (*1 Institute for Molecular Science)

第28回化学反応討論会 (春日), 2012年6月, 1P32

Dissociative photoionization of perfluorocyclobutane studied by mass-resolved photoion imagingKazumasa Okada^{*1}, Toru Nakashima^{*1}, Hideki Katayanagi^{*2}, Atsushi Suemitsu^{*1}, and Koichiro Mitsuke (*1 Hiroshima University, *2 Institute for Molecular Science)

第28回化学反応討論会 (春日), 2012年6月, 2P12

質量分解能を向上させた画像観測装置を用いた, フラーレン類の解離性光イオン化機構の解明片柳英樹^{*1}, 見附孝一郎 (*1 分子科学研究所)

第6回分子科学討論会 (東京), 2012年9月, 1P008

色素増感太陽電池の正極に用いる白金ナノ粒子の合成と評価河野 睦, アンジェリ レイ^{*1}, トンゴル ベルナルド^{*1}, 秋田素子, 見附孝一郎 (*1 サントトーマス大学)

第6回分子科学討論会 (東京), 2012年9月, 2P075

質量分解能を向上させた画像観測装置を用いたフラーレン類の解離性光イオン化機構の解明

片柳英樹^{*1}, 見附孝一郎 (*1 分子科学研究所)

UVSOR シンポジウム 2012 (岡崎), 2012 年 11 月

ルイス塩基として働くカルボン酸 (2) : 安息香酸銅 (II) ・安息香酸付加物の構造

宮前 博・林 瑛司・日原五郎

日本化学会第 92 春季年会(日吉), 2012 年 3 月, 講演予稿集, 2PA-268

PbX_2 (X=Cl or Br) に 2,3-bis(2-pyridyl)pyrazine で架橋されてできる二重シート構造

宮前 博・宮本 育代・日原 五郎

錯体化学第 62 回討論会(富山), 2012 年 9 月, 講演要旨集, p. 349 (2PB-010).

低温で淡色化を示した $[Ni(en)_2]_3[Ni(H_2O)_2(en)_2][Pb_2Cl_8]_2$ の結晶構造

宮前 博・東海林 了・日原 五郎

日本結晶学会年会(仙台), 2012 年 10 月, 講演要旨集, p. 89 (26-PB-02).

ハト羽毛ケラチン calamus 遺伝子のスクリーニング

高橋理恵子

第 85 回 日本生化学会大会(福岡), 2012 年 12 月, 講演要旨集, p. 113

クロシヨウジョウバエのペプチドグリカン認識タンパク-SC (PGRP-SC) の解析

北川浩子

第 85 回日本生化学会 (福岡), 2012 年 12 月

ミトコンドリア DNA 分析によるアユカケの遺伝的多様性

石黒直哉, 田原大輔^{*1} (*1 福井県大海洋生資)

日本 DNA 多型学会第 21 回学術集会 (京都), 2012 年 11 月, 抄録集, p. 54

天王川及び吉野瀬川におけるドジョウの遺伝的特性

日和佳政^{*1}, 藤長裕平^{*1}, 石黒直哉, 田原大輔^{*2} (*1 越前市農政課, *2 福井県大海洋生資)

日本 DNA 多型学会第 21 回学術集会 (京都), 2012 年 11 月, 抄録集, p. 57

Luminescent Quantum Dots and Plasmonic Metal Particles, Versatile Tools for Bioimaging

Itoh, T.*, Biju, V.*, Ishikawa, M. (*Health Research Institute, AIST, Shikoku)

The 7th Asian Photochemistry Conference 2012 (APC2012), 12-15 November 2012, Osaka University, Suita, Japan. *Invited Talk*

Fluctuation in Surface-Enhanced Raman Scattering and Surface-Enhanced Fluorescence of Single Plasmonic Metal Nanoparticle Dimer

T. Itoh,^{*1} Y. S. Yamamoto,^{*1} M. Iga,^{*1} H. Tamaru,^{*2} V. Biju,^{*1} M. Ishikawa, Y. Ozaki^{*3} (*1 Health Research Institute, AIST, Shikoku, *2 Department of Applied Physics, The University of Tokyo, *3 Department of Chemistry, Kwansai Gakuin University)

The 7th Asian Photochemistry Conference 2012 (APC2012), 12-15 November 2012, Osaka University, Suita, Japan.

Energy and electron transfer in quantum dots-based donor-acceptor systems

V. Biju,^{*1} E. S. Shibu,^{*1} M. Hamada,^{*1} N. Murase,^{*1} T. Itoh,^{*1} A. Furube,^{*2} M. Ishikawa, L. Wang,^{*3} S. Masuo,^{*3} N. Tamai^{*3} (*1 Health Research Institute, AIST, Shikoku, *2 Research Institute of Instrumentation Frontier, AIST, Tsukuba, *3 Department of Chemistry, Kwansai Gakuin University)

The 7th Asian Photochemistry Conference 2012 (APC2012), 12-15 November 2012, Osaka University, Suita, Japan.

Energy transfer-mediated photodecomposition of undesired acceptors to reversibly report the condensation and decondensation of DNA

V. Biju,^{*1} N. Murase,^{*1} E. S. Shibu,^{*1} T. Itoh,^{*1} H. Akita,^{*2} H. Harashima,^{*2} M. Ishikawa (*1 Health Research Institute, AIST, Shikoku, *2 Faculty of Pharmaceutical Sciences, Hokkaido University)

2012年光化学討論会, 東京工業大学大岡山キャンパス(2012/9/12-14)

フェムト秒レーザー照射に伴う水の多光子吸収を介した金 / 銀ナノ粒子作製

宇和田 貴之, 王 順發^{*1}, 増原 宏^{*1} (*1 台湾交通大学理学院化学科および分子科学研究所)

2012年光化学討論会, 東京工業大学 (東京都), 2012年9月

Gold/silver nanoparticles fabrication by femtosecond laser induced optical breakdown

Takayuki Uwada, Shun-Fa Wang^{*1}, Hiroshi Masuhara^{*1} (*1 Department of Applied Chemistry and Institute of Molecular Science, National Chiao Tung University, Taiwan)

International Conference on the Nanostructure-Enhanced Photo-Energy Conversion (Tokyo),
2012 年 6 月

Laser induced two-dimensional nanoparticle assembly formation in the vicinity of a single gold nanoparticle

Takayuki Uwada, Tzu-Wei Hsu^{*1}, Hiroshi Masuhara^{*1} (*1 Department of Applied Chemistry and Institute of Molecular Science, National Chiao Tung University, Taiwan)

International Conference on the Nanostructure-Enhanced Photo-Energy Conversion (Tokyo),
2012 年 6 月

金ナノ粒子トラッピングダイナミクスにおける熱対流の協奏効果

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単一金ナノ粒子のレーザー加熱による二次元ナノ粒子／分子集合体形成

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Laser trapping-induced reconfiguration of individual smectic liquid crystal micro-droplet showing size-dependent dynamics

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松坂卓也, 高崎祐人, 宮前智紀, 若林英嗣, 栗原照夫

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