

The Chemical Society of Japan The 95th Annual Meeting
Date March 27th, 2015
Venue Funabashi Campus, Nihon University, Chiba, Japan

COVAL SOCIETY The Royal Society of Chemistry



The Chemical Society of Japan

The 6th RSC-CSJ Joint Symposium

—Advanced Measurements for Chemistry—

The Chemical Society of Japan The 95th Annual Meeting

	Date March 27th (Fri), 2015 9:30-16:44	0	
	Venue Room 1423 (S5) 2nd Floor 14th Blo	lg.,	
	Funabashi Campus, Nihon University, Chiba	a, Japan	
	Hosted by The Chemical Society of Japan (CSJ)	
	Co-hosted by The Royal Society of Chemist	ry (RSC)	
■ 9:30	Opening Remarks	Robert Parker CEO; RSC	
■ 9:40	Ultrafast Studies of Reactive Dynamics by 1 and 2D Spectroscopy	Stephen R. Meech, et al. University of East Anglia	1
∎10:20	Femtosecond Time-Resolved Impulsive Stimulated Raman Spectroscopy of Complex Molecular Systems	Tahei Tahara RIKEN	3
∎11:00	Break		
∎11:10	Multiplexed and Quantitative Bioanalysis Using Surface Enhanced Raman Spectroscopy (SERS)	Karen Faulds University of Strathclyde	5
∎11:50	High-Speed Atomic Force Microscopy for Observation of Single-Molecule Dynamics	Takayuki Uchihashi Kanazawa University	7
∎12:30	Lunch Break		
■ 13:40	Novel Strategies in Single Molecule Sensing	Joshua B. Edel Imperial College London	9
∎14:20	Carrier Transport in Single Molecules	Hirokazu Tada Osaka University	11
∎15:00	Break		
∎15:10	New Analytical Tools for Aerosol Particles	Jonathan P. Reid University of Bristol	13
∎15:50	Chemical Evolution in Star and Planet Formation	Nami Sakai The University of Tokyo	15
∎16:30	Closing Remarks Signing Ceremony of the International Cooperation Agreement (RCS & CSJ)	Nobuyuki KAWASHIMA Excutive Director, CSJ Robert Parker CEO; RSC	

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Welcome Address

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Dear Colleagues,

Welcome to the 6th RSC-CSJ Joint Symposium, held at the same venue as the 95th CSJ Annual Meeting, Funabashi Campus, College of Science and Technology, Nihon University, Chiba, Japan on March 27th, 2015, under the co-sponsorship of



the Chemical Society of Japan (CSJ) and Royal Society of Chemistry (RSC).

Our prime mission is to contribute to social development through advancing science, developing technology, promoting industry, diffusion of knowledge relating to chemistry, and developing human resources. To pursue this mission, the CSJ holds various conferences, such as "the CSJ Annual Meeting" with 9,000 participants every spring, and "CSJ Chemistry Festa" every autumn.

This series of bilateral meetings originates from the first one in 2007 held at Osaka University, followed by the second in 2008 at Queen's University and the third in 2010 at the RSC Burlington House where we signed an International Cooperation Agreement between RSC and CSJ. The fourth and fifth symposia were held in 2012 at Ritsumeikan University and in 2014 in Dublin respectively.

"Advanced Measurements for Chemistry", the topic of the 2015 joint symposium is a highly advanced interdisciplinary field that covers from single molecule sensing to efforts to study the birth of stars and planets. Eight distinguished scientists in the area of advanced measurements are invited to present their research and to exchange information and ideas.

I would like to thank Co-Chairs Dr. Tahei Tahara, Riken and Prof. Stephen Meech, University East Anglia, and Dr. Sarah Thomas, RSC for their great efforts to make this symposium possible. It is my hope that this symposium will contribute to the rapid development of this field and I also have great expectations that all of the attendants will strengthen their friendships and find new colleagues throughout the symposium and the CSJ Annual Meeting for further collaboration.

Mr. Nobuyuki Kawashima

Executive Director / Secretary General The Chemical Society of Japan

Welcome Address

Dear Colleagues

Welcome to the sixth in our series of Joint Chemical Society of Japan (CSJ) and Royal Society of Chemistry (RSC) symposia. We are delighted to have this opportunity and thank Mr Nobuyuki Kawashima, CSJ Executive Director and Professor Tahei Tahara from RIKEN for all their help and support in organizing this event.

This symposium is one of the activities jointly organized following

the signing in 2010 of a five year International Cooperation Agreement between the CSJ and the RSC. Since the signing there have been many successful events including joint symposia in chemical biology and supramolecular chemistry, the annual awarding of the PCCP prize and participation in the high profile Chemical Sciences and Society Symposia series. We are delighted that we will be renewing our partnership with the CSJ at this meeting and re-signing our International Cooperation Agreement for a further five years. We very much look forward to many more successful joint activities in the coming years.

The Royal Society of Chemistry is the world's leading chemistry community, advancing excellence in the chemical sciences. With over 51,000 members and a knowledge business that spans the globe, we are the UK's professional body for chemical scientists, supporting and representing our members and bringing together chemical scientists from all over the world.

A not-for-profit organization with a heritage that spans 170 years, we have an ambitious international vision for the future. Around the world, we invest in educating future generations of scientists. We raise and maintain standards. We partner with industry and academia, promoting collaboration and innovation. We advise government on policy. And we promote the talent, information and ideas that lead to great advances in science.

In a complex and changing world, chemistry and the chemical sciences are essential. They are vital in our everyday lives and will be vital in helping the world respond to some of its biggest challenges. We're working to shape the future of the chemical sciences – for the benefit of science and humanity.

The RSC is also pleased to have the opportunity to work more closely with the Japanese chemical science community through Dr Hiromitsu Urakami, our Representative for Japan, who is based full-time in our office in Tokyo. This office is located in the CSJ building in Tokyo and we are very grateful to the CSJ for all their help and advice in establishing this office.

Each of the speakers in this symposium is an international expert in the area of investigating and applying advanced measurement methods in the chemical sciences. We hope that the presentations will stimulate the exchange of ideas and experiences between all participants. We thank each of the speakers and all the participants for their contributions to this symposium.

Once again a very warm welcome to what promises to be an exciting scientific event. We hope that the symposium will provide a springboard for future activities and that it will foster new research collaborations. We look forward to continuing our close partnership with CSJ, with more joint CSJ-RSC activities in the future.

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Dr Robert Parker Chief Executive Officer Royal Society of Chemistry

Stephen Meech

Professor of Physical Chemistry School of Chemistry, The University of East Anglia Address: Norwich NR4 7TK, UK Tel: (+44)-1603-593141 E-mail: S.Meech@uea.ac.uk



Educational Background

1978 B.Sc., Chemistry University of East Anglia1983 Doctor of Chemistry, University of Southampton (supervisor: Prof. David Philips)

Professional Career

1/1/82-1/1/83	Postdoctoral Research Associate, Wayne State University, Detroit, USA
1/1/83-1/10/84	Postdoctoral Research Associate, The Royal Institution, London
1/10/84-1/6/96	Royal Society/SERC Research Fellow, University of Groningen, The Netherlands.
1/6/86- 1/3/94	Lecturer in Chemistry, Heriot-Watt University, Edinburgh.
(1/10/88-1/1/90)	Inoue Research Fellow, Institute for Molecular Science, Japan.
1/3/94- 1/8/98	Lecturer in Chemistry, University of East Anglia, Norwich.
1/8/98 - 31/8/04	Reader in Physical Chemistry, University of East Anglia
1/9/04 - present	Professor of Physical Chemistry, University of East Anglia

Research Interests

1) Ultrafast Spectroscopy 2) Photoactive Proteins 3) Excited state dynamics

> Awards

- 1984 Royal Society European Research Fellowship
- 1984 SERC Post-doctoral Fellowship (declined)
- 1987 Inoue Science Foundation Fellowship
- 1993 Daiwa-Adrian Prize (With K. Yoshihara and J. G. Frey)
- 1995 JSPS fellowship
- 2001 JSPS fellowship
- 2007 RIKEN Visiting Senior Scientist

- 1.BLUF Domain Function Does Not Require a Metastable Radical Intermediate State, A. Lukacs, R. Brust, A. L. Haigney, S. P. Laptenok; K. Addison, A. Gil, G. M. Greetham, M. Towrie, P. J. Tonge, and S. R. Meech J. Am. Chem. Soc. 2014, 136, 4605. DOI: 10.1021/ja4121082
- Two-dimensional electronic spectroscopy based on conventional optics and fast dual chopper data acquisition, I. A. Heisler, R. Moca, F. V. A. Camargo, and S. R. Meech *Rev. Sci. Instrum.* 2014, 85, 063103 (10 pages). DOI: 10.1063/1.4879822
- 3.Excited State Structural Dynamics in Higher Lying Electronic States: S₂ State of Malachite Green, S. Laptenok, K. Addison, I. A. Heisler, and S. R. Meech, Chem. Phys. Lett. 2014, 607, 43. DOI: 10.1016/j.cplett.2014.05.050
- 4. Chemically Optimising Operational Efficiency of Molecular Rotary Motors, J. Conyard, A. Cnossen, W. R. Brown, B. L. Feringa, and S. R. Meech J. Am. Chem. Soc. 2014, 136, 9692. (Featured as a 'Spotlight article' 10.1021/ja506476x, J. Am. Chem. Soc. 2014, 136, 9519.) DOI: 10.1021/ja5041368
- Ultrafast Excited State Dynamics in 9,9'-Bifluorenylidene, J. Conyard, I. Heisler, W. R. Brown, B. L. Feringa, S. Amiirjalayer, S. Wouterson, W-J. Buma, and S. R. Meech J. Phys. Chem. A, 2014, 118, 5961. DOI: 10.1021/jp504391s



Ultrafast Studies of Reactive Dynamics by 1 and 2D Spectroscopy

Ismael A. Heisler, Franco V. A. Camargo, and Stephen R. Meech*

School of Chemistry, University of East Anglia, Norwich, NR4 7TJ, U.K.

Excited state reactions studied by ultrafast pump - probe experiments have provided some of our best insights into the dynamics of chemical reactions in solution. Electronic excitation by a short pulse of light places the molecule at an unstable point on the excited state potential energy surface, and the relaxation from that point can be observed in real time. In this presentation we will describe the two methods, ultrafast fluorescence up-conversion and two-dimensional electronic spectroscopy (2DES), which can be used to observe excited state structural evolution. The fluorescence experiment is used to probe excited state conformational change in a molecular rotor, while 2DES probes torsional motion in a linear linked porphyrin dimer. The effects of medium viscosity and molecular volume on the structural dynamic are investigated.



Figure 1. Projection of the time-resolved fluorescence of the molecular rotor, showing the rapid decay, red shift and coherent oscillations on the sub-picoseconf timescale.

Tahei Tahara

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Educational Background

1984 B.Sc., University of Tokyo (supervisor: Prof. Mitsuo Tasumi)

- 1986 M.Sc., Graduate School of Science, University of Tokyo (supervisor: Prof. Mitsuo Tasumi)
- 1989 Doctor of Science, Graduate School of Science, University of Tokyo (supervisor: Prof. Mitsuo Tasumi)

Professional Career

1989 Research Associate, The University of Tokyo

- 1990 Research Associate, Kanagawa Academy of Science and Technology
- 1995 Associate Professor, Institute for Molecular Science (IMS)
- 2001 Chief Scientist, Molecular Spectroscopy Laboratory, RIKEN

> Research Interests

ultrafast spectroscopy, nonlinear spectroscopy and single molecular spectroscopy of complex molecular systems

> Awards

- 1995 Research Foundation for Opto-Science and Technology Award
- 2000 Morino Science Award
- 2001 TRVS Outstanding Young Researcher Award
- 2004 IBM Japan Science Prize
- 2006 The JSPS Prize
- 2013 CSJ Award for Creative Work

- 1. Two-dimensional fluorescence lifetime correlation spectroscopy 1. Principle & 2. Application, K. Ishii and T. Tahara, J. Phys. Chem. B 2013, 117, 11414 & 11423.
- 2. Ultrafast vibrational dynamics of water at a charged interface revealed by two-dimensional heterodyne-detected vibrational sum frequency generation, P. C. Singh, S. Nihonyanagi, S. Yamaguchi, and T. Tahara, J. Chem. Phys. **2012**, 137, 094706.
- 3. Three distinct water structures at a zwitterionic lipid/water interface revealed by heterodyne-detected vibrational sum frequency generation, J. A. Mondal, S. Nihonyanagi, S. Yamaguchi, and T. Tahara, J. Am. Chem. Soc. **2012**, 134, 7842.
- Unified molecular view of air/water interface based on experimental and theoretical χ⁽²⁾ spectra of isotopically diluted water surface, S. Nihonyanagi, T. Ishiyama, T. Lee, S. Yamaguchi, M. Bonn, A. Morita, and T. Tahara, J. Am. Chem. Soc. 2011, 133, 16875.
- Coherent nuclear dynamics in ultrafast photoinduced structural change of bis(diimine) copper (I) complex, M. Iwamura, H. Watanabe, K. Ishii, S. Takeuchi, and T. Tahara, J. Am. Chem. Soc. 2011, 133, 7728.





Femtosecond Time-Resolved Impulsive Stimulated Raman Spectroscopy of Complex Molecular Systems

Tahei Tahara^{a,b}

^a Molecular Spectroscopy Laboratory, RIKEN, 2-1 Hirosawa, Wako 351-0198, Japan ^{b.} Ultrafast Spectroscopy Research Team, RIKEN Center for Advanced Photonics (RAP), 2-1 Hirosawa, Wako 351-0198, Japan

In ordinary Raman spectroscopy, we measure energetically-shifted inelastic light scattering, and the energy shift from the excitation light provides information of the vibrational transition energy of the molecule. However, by using ultrashort optical pulses that have duration shorter than the vibrational period, we can induce coherent nuclear motion of the molecule by the impulsive Raman process and observe Raman-active vibrations directly in the time domain. This way of Raman spectroscopy is called time-domain Raman spectroscopy.

Time-domain Raman spectroscopy is very useful for observing the molecular vibration of short-lived transients. For measuring time-resolved Raman spectra with femtosecond time resolution, we developed time-resolved impulsive stimulated Raman spectroscopy (TR-ISRS) and demonstrated its high potential to study excited-state molecules.^{1, 2} In this method, we use three femtosecond pulses: The first pulse (P1) photoexcites the molecule to start chemical reactions. The second pulse (P2) induces coherent nuclear wavepacket motion in the transient species, and the third pulse (P3) detects the wavepacket motion through the oscillation of the transient absorption and/or stimulated emission. The Fourier transforms of the observed oscillation give femtosecond time-resolved Raman spectra. Because we use only femtosecond pulses in the measurements, we can change the delay time with a femtosecond accuracy. Therefore, we can track the temporal change of the sample through the evolution of femtosecond time-resolved Raman spectra. We are now able to carry out TR-ISRS experiments using 6-fs optical pulses, which enables us to observe all the fundamental vibrational motions including CH stretch vibrations over 3000 cm⁻¹.

In this presentation, I report on our most recent TR-ISRS studies of a photoreceptor protein, photoactive yellow protein (PYP).³ The obtained femtosecond time-resolved Raman spectra clarified the initial events occurring after photoexcitation through the vibrations of key transient intermediates. It was concluded that the chromophore (p-coumaric acid) retains a trans-configuration in the excited pG^* state that appears immediately after photoexcitation while the surrounding hydrogen-bonding structure changes in a few hundred femtoseconds. Time-resolved

Raman spectra of the first ground-state intermediate (I_0 state) have also been measured with very high S/N. The comparison between the obtained Raman spectrum and DFT calculation indicates that the chromophore in the I_0 state has a highly distorted cis-form.

- 1. S. Fujiyoshi, S. Takeuchi, and T. Tahara, J. Phys. Chem. A 2003, 107, 494.
- S. Takeuchi, S. Ruhman, T. Tsuneda, M Chiba, T. Taketsugu, and T. Tahara, *Science* 2008, *322*, 1073.
- 3. H. Kuramochi, S. Takeuchi, K. Yonezawa, H, Kamikubo, M. Kataoka, and T. Tahara, in preparation (2015).



Figure 1. Experimental Scheme of TR-ISRS.

Karen Faulds

BSc(Hons), PhD, PgCert, FRSC, FHEA

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Educational Background

- 1998 BSc(Hons) Forensic and Analytical Chemistry, University of Strathclyde
- 2003 PhD, Detection of Drugs of Abuse by SERS, University of Strathclyde (Prof W. E. Smith)
- 2008 PgCert., Advanced Academic Studies, University of Strathclyde

Professional Career

- 2003 Postdoctoral Researcher (DTI, LGC), University of Strathclyde
- 2004 Postdoctoral Researcher (BBSRC), University of Strathclyde
- 2006 Lecturer in Bioanalytical Chemistry, University of Strathclyde
- 2010 Senior Lecturer, University of Strathclyde
- 2012 Reader, University of Strathclyde

Research Interests

Our research focuses on using surface enhanced Raman scattering (SERS) to create new approaches to bioanalysis for use in the life and clinical sciences.

1) Using the inherent sensitivity of SERS for the detection of target DNA or proteins using signal amplification methods to enhance the signal rather than using target amplification methods.

2) Exploiting the sensitivity of SERS for quantitative analysis of biomolecules as well as exploiting one of the key advantages of SERS, the ability to analyse multiple analytes in one sample.

> Awards

- 2009 Nexxus 2009 Young Life Scientist of the Year Award
- 2009 Awarded Fellowship of the Higher Education Academy status (FHEA)
- 2012 Elected to the Royal Society of Edinburgh's Young Academy of Scotland
- 2012 Elected Fellow of the Royal Society of Chemistry (FRSC)
- 2013 RSC Joseph Black Award

- 1. *Simultaneous Detection and Quantification of Three Bacterial Meningitis Pathogens by SERS*, Gracie K, Correa E, Mabbott S, Dougan JA, Graham D, Goodacre R, and Faulds K*, *Chem. Sci.* **2014**, 5(3), 1030.
- 2. *Resonance Raman scattering of catalytic beacons for DNA detection*, McKeating KS, Graham D, and Faulds K*, *Chem. Commun.* **2013**, 49 (31), 3206.
- 3. Specific detection of DNA through coupling of a TaqMan assay with surface enhanced Raman scattering (SERS), Harper MM, Robertson B, Ricketts A, and Faulds K*, *Chem. Commun.* **2012**, 48 (75), 9412.
- 4. *DNA Detection Using Enzymatic Signal Production and SERS*, Dougan JA, MacRae D, Graham D, and Faulds K*, Chem. Commun. **2011**, 47 (16), 4649.





Multiplexed and Quantitative Bioanalysis Using Surface Enhanced Raman Spectroscopy (SERS)

K. Faulds,^{*a} K. Gracie,^a E. Correa,^b S. Mabbott,^a J. A. Dougan,^a D. Graham,^a R. Goodacre,^b and S. McAughtrie^a

^aCentre for Nanometrology, WestCHEM, Department of Pre and Applied Chemistry, University of Strathclyde, 295 Cathedral Street, Glasgow, G1 1XL, U.K. ^bSchool of Chemistry and Manchester Interdisciplinary Biocentre, University of Manchester, 131 Princes Street, Manchester, M1 7ND, U.K.

Surface enhanced Raman scattering (SERS) is an analytical technique with several advantages over competitive techniques in terms of improved sensitivity and multiplexing. We have made great progress in the development of SERS as a quantitative analytical method, in particular for the detection of DNA. However, the lack of quantitative data relating to real examples has prevented more widespread adoption of the technique. Detection of specific DNA sequences is central to modern molecular biology and also to molecular diagnostics where identification of a particular disease is based on nucleic acid identification. Many methods exist and fluorescence spectroscopy dominates the detection technologies employed with different assay formats. Another advantage of SERRS over existing detection techniques is that of the ability to multiplex which is limited when using techniques such as fluorescence. We have clearly demonstrated the ability to identify the presence of a mixture of 6 analytes in solution using data analysis techniques.

Here we demonstrate the development of new molecular diagnostic assays based upon SERS which have been used successfully for the detection of bacterial pathogens associated with meningitis using modified SERS active probes. The probes have been designed to give a specific SERS response resulting in discernable differences in the SERS which can be correlated to a specific DNA hybridisation event. In this presentation the simultaneous detection and quantitation of 3 pathogens within a multiplex sample will be demonstrated for the first time.

We also have an interest in the development of functionalised nanoparticles as sensing materials for the detection of DNA at ultra low levels, proteins and more recently as substrates for imaging approaches. We achieve this by combining functionalised silver or gold nanoparticles with SERS. This combination can result in extremely sensitive and selective biosensing with unprecedented multiplexing capabilities. This approach has been extended to look at the multiplexed, 3D imaging of functionalised nanoparticles in cells.

Takayuki Uchihashi

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Educational Background

- 1993 B.Sc., Department of Physics, Hiroshima University (supervisor: Prof. Seizo Morita)
- 1995 M.Sc., Graduate School of Physics, Hiroshima University (supervisor: Prof. Seizo Morita)
- 1998 PhD in Engineering Graduate School of Engineering, Osaka University (supervisor: Prof. Seizo Morita)

Professional Career

- 1998 Research associate, Joint Research Center for Atom Technology
- 2000 Assistant professor, Himeji Institute of Technology
- 2002 Senior Scientist, SFI Nanoscience Laboratory, Trinity College, Dublin
- 2004 Assistant professor, Kanazawa University

2006 Associate Professor, Kanazawa University

Research Interests

1) Single-molecule observations for revealing molecular mechanisms of protein function

2) Development of novel probe microscopy techniques

> Awards

2006 The 29th JJAP Paper Award by Japanese Society of Applied Physics

- 2010 Nanoprobe Technology Award by JSPS the 167th committee
- 2013 The Commendation for Science and Technology by the Minister of Education, Culture, Sports, Science and Technology, Development Category

- 1. Probing structural dynamics of an artificial protein cage using high-speed atomic force microscopy, M. Imamura, T. Uchihashi et al., Nano Lett. (in press).
- 2. *Filming biomolecular processes by high-speed atomic force microscopy*, T. Ando, T. Uchihashi, and S. Scheuring, *Chem. Rev.* **2014**, *114*, 3120.
- 3. *Two-way traffic of glycoside hydrolase family 18 processive chitinases on crystalline chitin,* K. Igarashi, T. Uchihashi et al., *Nat. Commun.* **2014**, *5*, 3975.
- 4. Traffic jams reduce hydrolytic efficiency of cellulose on cellulose surface, K. Igartashi, T. Uchiashi et al., Science **2011**, 333, 1279.
- 5. High-speed atomic force microscopy reveals rotary catalysis of rotorless F_1 -ATPase, T. Uchihashi, R. Iino et al., Science **2011**, 333, 755.



High-Speed Atomic Force Microscopy for Observation of Single-Molecule Dynamics

TAKAYUKI Uchihashi, $^{\mathrm{a,b,c}}$ NORIYUKI Kodera $^{\mathrm{b,d}}$ and TOSHIO Ando $^{\mathrm{a,b,c}}$

^aDepartment of Physics, Kanazawa University, Kanazawa, Ishikawa 920-1192, Japan ^bBio-AFM Frontier Research Center, Kanazawa University, Kanazawa, Ishikawa 920-1192, Japan ^cJST-CREST, 4-1-8 Hon-cho, Kawaguchi, Saitama 332-0012, Japan ^dJST-PREST, 4-1-8 Hon-cho, Kawaguchi, Saitama 332-0012, Japan

Conventional techniques such as X-ray crystallography, electron microscopy and nuclear magnetic resonance have been successful in determining the protein 3D structure at even atomic level. However, the obtainable structure is a static one averaged over many molecules and hence cannot directly reveal how protein molecules behave dynamically when they are functioning in solution. Currently-prospering single molecule analysis by fluorescence microscopy can detect dynamic behavior of protein at work but the spatial resolution is not high enough to visualize protein structure. Atomic force microscopy (AFM) does not possess spatial resolution as high as other techniques but very unique in its ability to visualize individual protein molecules in solution at (sub) nanometer resolution. However, its imaging rate was too low to capture dynamically moving molecules because of the slow scan speed due to the slow mechanical responses of the cantilever and scanner. In addition, large tip-sample interaction often disturbs weak protein-protein interactions and even leads to destruction of fragile proteins.

In order to afford AFM to trace moving protein molecules without disturbing their physiological function, we have been developing various devices over the past decade. Finally the imaging speed of AFM has been improved to be 10-30 frames/s. The high-speed AFM capture dynamic events of various proteins without significantly disturbing week biomolecular interaction. For instance, the following dynamics have been successfully captured on video; dynamics of bacteriorhodopsin 2D crystals,¹ myosin V walking on an actin filament,² conformational change of bacteriorhodopsin in response to light,³ rotary catalysis of rotorless F₁-ATPase⁴ and cellulase hydrolyzing crystalline cellulose fibers.⁵ These demonstrations clearly indicate that high-speed AFM has a great potential of giving straight and quick answers to how and what structural changes of individual molecules progress while their physiological function is being produces.

In this talk, I briefly introduce key techniques enabling fast scanning of AFM and demonstrate some high-speed AFM movies to show its capability for studying dynamic biomolecular processes.

References

- 1. H. Yamashita et al., J. Struct. Biol. 2009, 97, 2358.
- 2. N. Kodera, D. Yamamoto, R. Ishikawa, and T. Ando, *Nature* 2010, 468, 72.
- 3. M. Shibata et al., Nat. Nanotech. 2010, 5, 208.
- 4. T. Uchihashi, R. Iino, T. Ando, and H. Noji, Science 2011, 333, 755.
- 5. K. Igarashi et al., *Science* **2011**, *333*, 1279.

Joshua B. Edel

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Educational Background

10/00 – 12/03: **Ph.D. in physical chemistry**.Imperial College London. (University of London, UK). 09/96 – 07/00: **B.Sc. (Hon.) in chemistry**. University of British Columbia. (Vancouver, Canada).

- **Research Experience**
- 2014 Reader in (Bio)Sensing and Analytical Sciences
- 2009 Senior Lecturer in micro and nanotechnology
- 2006 2009 Lecturer in micro and nanotechnology Institute of Biomedical Engineering and Department of Chemistry Imperial College London, UK
- 2005 2006 Postdoctoral research fellow with Prof. Amit Meller. Rowland Institute at Harvard, Harvard University, USA. *Research focus:* Single molecule fluorescence lifetime imaging of DNA constructs
 2004 2005 Postdoctoral research especiate with Prof. Harold Craighead
- 2004-2005 **Postdoctoral research associate** with <u>Prof. Harold Craighead.</u> School of Applied and Engineering Physics, Cornell University, USA. *Research focus:* Development of nanofluidic and nano-optical devices for molecular separation and detection
- Recent Publications (out of a total of 85 journal articles, 10 patents/applications, 55 refereed conference proceedings, h-index (Google scholar) = 31)
- Precise Attolitre Temperature Control of Nanopore Sensors Using a Nanoplasmonic Bullseye, C. R. Crick, P. Albella, B. Ng, A. P. Ivanov, T. Roschuk, M. P. Cecchini, F. Bresme, S. A. Maier, and J. B. Edel*Nano Lett. 2015, 15(1), 553, DOI: 10.1021/nl504536j
- Single Molecule Sensing with Solid-state Nanopores: Novel Materials, Methods, and Applications, B. N. Miles, A. P. Ivanov, K. A. Wilson, F. Doğan, D. Japrung, and J. B. Edel, Chem. Soc. Rev.2013. 42, 15. DOI: 10.1039/C2CS35286A
- 3. Self-assembled nanoparticle arrays for multiphase trace analyte detection, M. P. Cecchini, V. A. Turek, J. Paget, A. A. Kornyshev,* and J. B. Edel,* *Nat. Mater.* **2013**, *12*, 165. **DOI**: 10.1038/nmat3488.
- 4. *A microdroplet dilutor for high-throughput screening*, X. Niu, F. Gielen, J. B. Edel,* and A. J. deMello,* *Nat. Chem.* **2011**, *3*, 437. (Cover Article). DOI:10.1038/nchem.1046
- DNA Tunneling Detector Embedded in a Nanopore, A. P. Ivanov, E. Instuli, C. M. McGilvery, G. Boldwin, D. W. McComb, T. Albrecht,* and J. B. Edel,* Nano Lett. 2011, 11(1), 279. DOI: 10.1021/nl103873a (Top 20 over 12 months).
- Plasmonic Ruler at the Liquid–Liquid Interface, V. A. Turek, M. P. Cecchini, J. Paget, A. R. Kucernak, A. A. Kornyshev,* and J. B. Edel,* ACS Nano 2012, 6(9), 7789. DOI: 10.1021/nn302941k
- Heavy Metal Sensing Using Self-Assembled Nanoparticles at a Liquid–Liquid Interface, M. P. Cecchini, V. A. Turek, A. Demetriadou, G. Britovsek, T. Welton, A. A. Kornyshev, D. E. T. Wilton-Ely, and J. B. Edel, DOI: 10.1002/adom.201400211



Novel Strategies in Single Molecule Sensing

Joshua B. Edel

Department of Chemistry, Imperial College London, Exhibition Road, SW& 2AZ, London U. K.

Analytical Sensors plays a crucial role in today's highly demanding exploration and development of new detection strategies. Whether it be medicine, biochemistry, bioengineering, or analytical chemistry the goals are essentially the same: 1) improve sensitivity, 2) maximize throughput, 3) and reduce the instrumental footprint. In order to address these key challenges, the analytical community has borrowed technologies and design philosophies which has been used by the semiconductor industry over the past 20 years. By doing so, key technological advances have been made which include the miniaturization of sensors and signal processing components which allows for the efficient detection of nanoscale object. One can imagine that by decreasing the dimensions of a sensor to a scale similar to that of a nanoscale object, the ultimate in sensitivity can potentially be achieved - the detection of single molecules. This talk highlights novel strategies for the detection of single molecules using multiphase microfluidics.

Relevant Papers

- Precise Attolitre Temperature Control of Nanopore Sensors Using a Nanoplasmonic Bullseye, C. R. Crick, P. Albella, B. Ng, A. P. Ivanov, T. Roschuk, M. P. Cecchini, F. Bresme, S. A. Maier, and J. B. Edel*Nano Lett. 2015, 15(1), 553, DOI: 10.1021/nl504536j
- 2. Single Molecule Ionic Current Sensing in Segmented Flow Microfluidics, T. R. Gibb, A. P. Ivanov, J. B. Edel, and T. Albrecht, Anal. Chem. **2014**, 86(3), 1864. **DOI**: 10.1021/ac403921m
- Rapid Ultrasensitive Single Particle Surface-Enhanced Raman Spectroscopy Using Metallic Nanopores, M. P. Cecchini, A. Wiener, V. A. Turek, H. Chon, S. Lee, A. P. Ivanov, D. W. McComb, J. Choo, T. Albrecht, S. A. Maier, and J. B. Edel, Nano Lett. 2013, 13(10), 4602. DOI: 10.1021/nl402108g
- 4. Single Molecule Sensing with Solid-state Nanopores: Novel Materials, Methods, and Applications, B. N. Miles, A. P. Ivanov, K. A. Wilson, F. Doğan, D. Japrung, and J. B. Edel, *Chem. Soc. Rev.*2013. 42, 15. DOI: 10.1039/C2CS35286A

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Educational Background

1982-1986,	Undergraduate Course, (supervisor: Prof. Kozo Kuchitsu)	
1986-1988,	Master Course, (supervisor: Prof. Kozo Kuchitsu)	
1998-1999,	PhD Course, (supervisor: Prof. Atsushi Koma)	
2003,	Doctor of Science	
	Department of Chemistry, School and Graduate School of Science,	
	The University of Tokyo	

Professional Career

1989-1993,	Assistant Professor, Dept. of Chem., School of Science, The University of Tokyo
1993-1996,	Senior Researcher, Commun. Res. Laboratory, Ministry of Posts and Telecommun.
1996-2000,	Lecturer, Dept. of Electronic Engineering Science, Graduate School of
	Engineering, Kyoto University
2000-2005,	Associate Professor, Inst. for Molecular Science, Okazaki National Institutes of
	Science

Research Interests

1) Molecular-based electronics, spintronics and thermoelectronics

2) Molecular-scale electronics, spintronics and thermoelectronics

- 1. *Magnetoluminescence of light-emitting field-effect transistors based on alpha sexithiophen*, S. T. Pham and H. Tada, *Appl. Phys. Lett.* **2014**,*104*, 133301.
- 2. Solution-processable n-Type Semiconducting Materials Containing a Carbonyl-bridged Thiazole-fused π System, Y. Ie, C. Sato, M. Nitani, H. Tada, and Y. Aso, Chem. Lett. **2014**, 43, 1640.
- 3. *Thermopower of Benzenedithiol and C60 Molecular Junctions with Ni and Au Electrodes*, S. K. Lee, T. Ohto, R. Yamada, and H. Tada, *Nano Lett.* **2014**, *14*, 5276.
- 4. Organic Magnetoresistance in Ambipolar Field-effect Transistor, S. T. Pham, Y. Kawasugi, and H. Tada, *Appl. Phys. Lett.* **2013**, *103*, 143301.
- 5. *Room-temperature magnetoresistance in organic spin-valves based on a Co2MnSi Heusler alloy*, Y. Kawasugi, T. Ujino, and H. Tada, *Org. Electron.* **2013**, *14*, 3186.





Carrier Transport in Single Molecules

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The concept of "molecular rectifier" proposed by Aviram and Ratner in 1974 (*Chem. Phys. Lett. 29*, 277) has motivated many researchers to prepare electronic devices based on single molecules. The break-junction method established in 2000s, illustrated schematically in Figure 1, has enabled us to carry out the quantitative measurement not only of electrical conductivity of single molecules inserted between metal electrodes, but also of transport properties of spins and heat in single molecular junctions. Various studies have acquired the deep knowledge concerning the origin of structural fluctuation and/or noise in the system, which encourages us to prepare novel devices with unique functions.



Figure 1. Preparation of metalmolecule-metal junctions using a break-junction method.

Figure 2a shows the thermoelectric voltage of Au-C60-Au and Ni-C60-Ni as a function of ΔT . Both junctions showed negative slope, which means a negative S. The result indicates that charge transport for C60 is through the LUMO level when using either Ni or Au as electrode. Seebeck coefficient of benzenedithiol (BDT) was positive and negative with Au and Ni electrodes, respectively (Figure 2b). We have investigated the result using the first-principle calculation and found that the spin splitting of HOMO of BDT occurs at the junction with Ni electrode.



Figure 2. Thermoelectric voltage as a function of ΔT for (a) C60 and (b) BDT molecular junctions.

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Educational Background

1994 M.Sc., University of Oxford, U.K.

1997 D. Phil., Department of Chemistry, University of Oxford (supervisor: Dr. C.J.S.M. Simpson)

Professional Career

- 1997 Post-doctoral research associate, JILA, University of Colorado, USA (supervisor: Prof. Stephen Leone)
- 2000 Lecturer in Physical Chemistry, Birmingham University
- 2004 Lecturer in Physical Chemistry, University of Bristol
- 2006 Reader in Physical Chemistry, University of Bristol
- 2009 Professor of Physical Chemistry, University of Bristol

Research Interests

- 1) Optical trapping and spectroscopy of single aerosol particles
- 2) Aerosols in the atmosphere, drug delivery and combustion

> Awards

- 2001 Harrison Memorial Prize of the Royal Society of Chemistry
- 2004 EPSRC Advanced Research Fellowship
- 2004 Marlow Medal of the Faraday Division of the Royal Society of Chemistry
- 2009 EPSRC Leadership Fellowship
- 2013 Corday-Morgan Prize of the Royal Society of Chemistry

- 1. Probing the Micro-Rheological Properties of Aerosol Particles using Optical Tweezers, R. M. Power and J. P. Reid, *Rep. Prog. Phys.* **2014**, *77*, 074601.
- 2. Measurements of the evaporation and hygroscopic response of single fine-mode aerosol particles using a Bessel beam optical trap, M. I. Cotterell, B. J. Mason, A. E. Carruthers, J. S. Walker, A. J. Orr-Ewing, and J. P. Reid, Phys. Chem. Chem. Phys. **2014**, *16*, 2118.
- The Influence of Organic Films on the Evaporation and Condensation of Water in Aerosol, J. F. Davies, R. E. H. Miles, A. E. Haddrell, and J. P. Reid, Proc. Natl. Acad. Sci. 2013, 110, 8807.
- 4. *The Transition from Liquid to Solid-Like Behaviour in Ultrahigh Viscosity Aerosol Particles*, R. M. Power, S. H. Simpson, J. P. Reid, and A. J. Hudson, *Chem. Sci.* **2013**, *4*, 2597.



New Analytical Tools for Aerosol Particles

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Aerosols find application in a broad range of scientific disicplines including combustion, drug delivery and spray drying. Atmospheric aerosols have a significant impact on the chemical composition of the atmosphere, on the radiative balance through scattering and absorbing light, and on the environment and health. Spanning in diameter from the nanometer to the 10's micrometres scale, new analytical tools are required to characterize the properties of aerosol and the factors that govern the processes they undergo over a wide range of lengthscales and timescales. Interfacial transport at the molecular level may occur on a timescale of nanoseconds, coalescence on a timescale of microseconds, condensation and evaporation on the millisecond to second timescale, and heterogeneous chemical aging on a timescale of hours or days. We will describe a range of novel optical techniques that probe aerosol properties and processes over a wide range of particle sizes and over timescales spanning form nanoseconds to days. These tools rely on trapping individual particles or arrays of particles in an optical trap or an electrodynamic balance. In particular, we will describe new methods for the following measurements:

- (1) Viscosity: By coalescing pairs of droplets and measuring the timescale for relaxation to a sphere, we will show that the viscosity of particles can be determined spanning the range 10^{-3} to 10^{9} Pa s, an exceptionally wide dynamic range.
- (2) Surface tension: From the relaxation timescale for coalescing pairs of droplets of low viscosity, we will also show that the surface tension of solution droplets can be inferred with high accuracy.
- (3) Evaporation/condensation kinetics: Measurements of the evolving size of droplets can be made with a time resolution of <10 ms, providing insights into the the highly dynamic nature of aerosol, including the impact of organic surface films on mass and heat transport in evaporating droplets.
- (4) Optical extinction and refractive index: The evolving extinction cross-sections can now be made on individual particles over an indefinite period of time, leading to highly accurate measurements of refractive index that can improve our understanding of scattering and absorption of light in the atmosphere.

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Educational Background

- 2004 B.Sc., Waseda University (supervisor: Prof. Daishido)
- 2006 M.Sc., Department of Physics, Graduate School of Science, The University of Tokyo (supervisor: Prof. Yamamoto)
- 2008 Ph.D., Department of Physics, Graduate School of Science, The University of Tokyo (supervisor: Prof. Yamamoto)

Professional Career

- 2007 JSPS Research Fellow for Doctoral course students (DC2)
- 2008 Assistant professor, Department of Physics, Graduate School of Science, The University of Tokyo

Research Interests

- 1) Star and planet formation
- 2) Astrochemistry

> Awards

2009 Inoue Research Award for Young Scientists

2013 ASJ (Astronomical Society of Japan) Research Award for Young Scientists

- 1. A Chemical View of Protostellar-Disk Formation in L1527, Sakai, N., et al. Astrophys. J. 2014, 791, L38.
- 2. Change in the Chemical Composition of Infalling Gas Forming a Disk around a Protostar, Sakai, N., et al. Nature **2014**, 507, 78.
- 3. Warm Carbon-Chain Chemistry, Sakai, N. and Yamamoto, S. Chem. Rev. 2013, 113, 8981.
- Anomalou ¹³C Isotope Abundances in C₃S and C₄H Observed toward the Cold Interstellar Cloud, Taurus Molecular Cloud-1, Sakai, N., Takano, S., Sakai, T., Shiba, S., Sumiyoshi, Y., Endo, Y., and Yamamoto, S. J. Phys. Chem. 2013, 117, 9831.



Chemical Evolution in Star and Planet Formation

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Star and planet formation is one of the most fundamental structure-formation processes in the Universe. Physical processes of star and planet formation have widely been investigated as one of the major targets of astronomy and astrophysics by observations in the entire wavelength region during the last few decades. Although a rough outline of these processes has been presented, there still remain many unknowns and missing links. One of them is when the disk structure is formed around a protostar, and how it is evolved into a protoplanetary disk and eventually to a planetary system. At the same time, understanding the evolution of matter from interstellar clouds to stars and planets is also a goal of astronomy. So far, about 180 interstellar molecules have been identified mainly by radio-astronomical observations, and about 1/3 of them are "complex" molecules having 6 atoms or more. This indicates the high chemical complexity of interstellar clouds even in the extreme condition of low temperature (10-100 K) and low density (10^2-10^7 cm⁻³) in comparison with the terrestrial condition, which would ultimately be related to an origin of rich substances in the Solar System. Thus, approaches both from physical and chemical view points are indispensable to bridge star/planet formation studies and planetary science of the Solar System.

In the last decade, it is clearly demonstrated that envelopes of solar-type protostars harbor various "complex" organic molecules (COMs) such as HCOOCH₃, (CH₃)₂O, and C₂H₅CN in the vicinity of the protostar. This result attracted much attention of astronomers and planetary scientists in relation to the origin of pre-solar organic materials found in meteorites and comets. On the other hand, protostellar envelopes which do not harbor COMs have also been found. Those sources are rich in carbon-chain molecules and their related species instead. Thus, now we know that there are at least two distinct families in chemical compositions; one is a hot corino characterized by abundant saturated COMs, whereas the other is a warm-carbon-chain-chemistry (WCCC) source characterized by abundant unsaturated COMs such as carbon-chain molecules and their related molecules. The chemical diversity would originate from different duration time of the starless core phase of each protostar. On the other hand, the most interesting issue to be studied is how the chemical diversity in the protostellar envelopes is brought into the later stages toward protostellar/protoplanetary disks. Fortunately, such a study is now feasible with high-sensitivity and high-angular-resolution capabilities of ALMA (Atacama Large Millimete/Submillimeter Array). ALMA is a large radio interferometer constructed at the high altitude site (5000 m) in Chile, which consists of 66 antennae in total. It is the most powerful radio telescope ever built, whose sensitivity and angular resolution are at least higher than the other telescopes by 2 orders of magnitude. Its early science operation was started with 16 antennae in 2011 (Cycle 0), and the full operation is coming soon. In this talk, I present importance of chemistry in astronomical studies by introducing chemical evolution from starless clouds to star forming clouds. I also talk about a drastic chemical change associated with disk formation, which was recently found with the ALMA observations.