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2nd WPI-Workshop
on Materials Science



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Nitride nanowire light emitting diodes: from single wire properties to flexible light emitters

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In this presentation we will review the forefront research on semiconductor nanowire light emitting diodes with a special attention to nitride materials emitting in the green and blue spectral range. We will show that these nanomaterials have the potential to boost the device performance, to improve the energy efficiency, to reduce the cost and to bring new functionalities. In particular, we will discuss our recent advances towards flexible nitride nanowire devices. We propose a method to combine high flexibility of polymer films with high quantum efficiency provided by nitride nanowires to achieve flexible inorganic light emitting diodes. We will also discuss the fabrication and characterization of single nanowire light emitting diodes with graphene transparent contacts [1] as well as the coupling of single nanowire emitters with waveguides in order to form a functional photonic platform [2].

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[2] Tchernycheva M., Messanvi A., de Luna Bugallo A., Jacopin G., Lavenus P., Rigutti L., Zhang H., Halioua Y., Julien F. H., Eymery J., Durand C., Integrated Photonic Platform Based on InGaN/GaN Nanowire Emitters and Detectors, *Nano Letters* 14, 3515 (2014).

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Fields of Research

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- *Nanowire-based photodetectors and light emitting diodes*
- *Nanowires for photovoltaic and piezoelectric conversion*
- *Intersubband devices based on GaN/AlN quantum wells and quantum dots*

Publications

- L. Rigutti and **M. Tchernycheva**, “Electrical and electro-optical characterization of semiconductor nanowires” pp. 641-85 in the 2nd edition of “Characterization of Semiconductor Heterostructures and Nanostructures”, Edited by C. Lamberti and G. Agostini, Elsevier (2013).
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- **Tchernycheva M**, Lavenus P, Zhang H, Babichev A V, Jacopin G, Shahmohammadi M, Julien F H, Ciechonski R, Vescovi G, Kryliouk O, InGaN/GaN Core-shell Single Nanowire Light Emitting Diodes with Graphene-Based P-Contact, *Nano Letters* 14, 2456 (2014).

Plasmonic Nanoarchitectonics for Energy Conversion

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Plasmonics and metamaterial are the new emerging paradigms for materials science which enable us to control the light in nano-space. Through this concept we have been developing materials with extraordinary signal enhancement of molecules, enhanced photocatalytic reaction, and efficient solar power harvesting. Currently, increasing interest exists in the field of solar heat energy conversion as well as in molecular sensing. Thanks to the rapid improvements in the bottom-up and top-down nanofabrication techniques in the past decade, dramatic progresses have been achieved in this field. Here in our laboratory we aim at manipulating the infrared light waves for enhancing the applications in environmental monitoring as well as solar and thermal energy conversion by developing new metallic and metallodielectric nano-structures. In this talk I will present some of the fundamental aspects and advantages of plasmonic resonators with both narrow-band and broad-band optical response, with emphasis on the dimensionality effects and nanogap geometry. Plasmonic nano-absorbers offers chances to realize high-efficiency light absorption with flexible spectrum engineering. In this talk, we report our recent research on the fabrication and characterization of plasmonic light scavengers/absorbers for the potential application in photocatalysis, plasmon-enhanced vibrational sensing for in situ water sensing, as well as light-heat transducers. Here we will exemplify nanogap-based molecular sensors and three dimensional broadband light absorbers/scatterers prepared by wet chemistry as well as lithographic fabrication. Together with numerical electromagnetic simulations, we showcase various fabrication methods using electron-beam lithography, photolithography, as well as colloidal templating process and nano-mechanical process for the large-area fabrication.

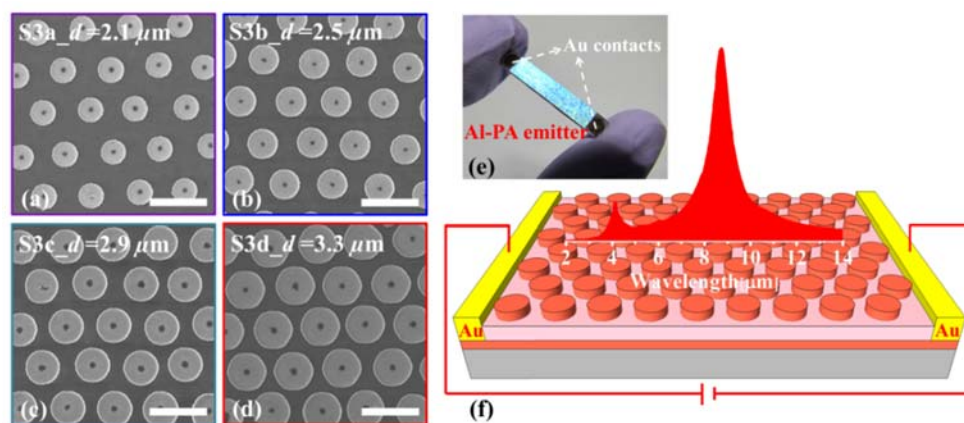


Figure. (a-d) SEM images of the metamaterial perfect absorbers. The scale bar in each image is $5 \mu\text{m}$. (e) A photo of a typical metamaterial thermal emitter device. (f) Schematic of a thermal emitter device having two Au electrodes.

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Publications

1. Thang Duy Dao, Gui Han, Nono Arai, Toshihide Nabatame, Yoshiki Wada, Chung Vu Hoang, Masakazu Aono and **Tadaaki Nagao**, "Plasmon-mediated photocatalytic activity of wet-chemically prepared ZnO nanowire arrays," Phys. Chem. Chem. Phys. **17**, 7395-7403 (2015).
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4. Jung-Sub Wi, Satoshi Tominaka, and **Tadaaki Nagao**, "Arrays of Nanoscale Gold Dishes Containing Engineered Substructures," Advanced Optical Materials **1**[11], 814-818(2013).
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Symmetric [111] grown GaAs droplet dots for quantum optics and spintronics

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Due to spatial confinement in all 3 dimensions, the energy states of an electron trapped inside a nano-crystal called Quantum Dot (QD) are discrete, in strong analogy to discrete energy states in atoms. We are able today to address and manipulate the quantum state of a single electron, in particular his spin state, confined in the dot in optical spectroscopy experiments [1].

InAs QDs in a GaAs matrix represent a model system for strain driven QD formation (Stransky-Krastanov growth mode) using Molecular Beam Epitaxy (MBE). Although technical progress has been impressive, this growth method has its limits: First, not all technical useful QD / barrier material combinations with different lattice constants can be grown. Second, growth along the crystallographic axis like 111 for symmetric quantum emitters is not possible. These problems can be overcome by an alternative growth method: In this talk we present work on GaAs QDs grown by **droplet epitaxy** in an MBE machine at the NIMS, Tsukuba by the group that invented this growth technique [2].

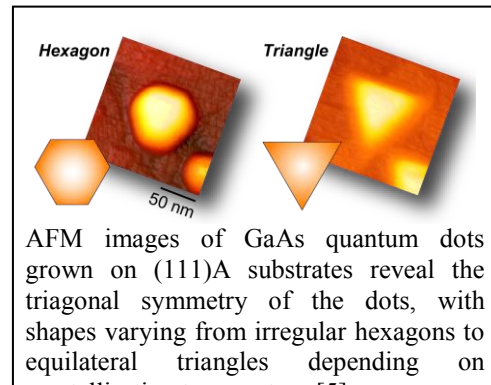
We demonstrate charge tuning in **strain free** GaAs/AlGaAs QDs grown on a GaAs(111)A substrate [3]. Application of a bias voltage allows the controlled charging of the QDs from $-3|e|$ to $+2|e|$. The resulting changes in QD emission energy and exciton fine-structure are recorded in micro-photoluminescence experiments at $T=4\text{K}$. We investigate optical pumping of the electron and also nuclear spins of the Ga and As atoms that form the dot in this system with a strong hyperfine interaction [1] and fascinating magneto-optical properties [4-6].

We also show that these symmetric 111 grown QDs can be used as efficient sources of highly entangled photons [7]. The emitted photons reveal a fidelity to the Bell state as high as 86 % without postselection. We show a violation of Bell's inequality by more than five times the standard deviation, a prerequisite to test a quantum cryptography channel for eavesdropping. The remaining decoherence channels of the photon source are ascribed to random charge and nuclear spin fluctuations in and near the dot.

We acknowledge partial funding from ERC project 306719.

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“Giant Enhancement of the Optical Second-Harmonic Emission of WSe₂ Monolayers by Laser Excitation at Exciton Resonances”

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Physical Review Letters 114, 097403 (2015)

“Charge tuning in [111] grown GaAs droplet quantum dots”

L. Bouet, M. Vidal, T. Mano, N. Ha, T. Kuroda, M. V. Durnev, M. M. Glazov, E. L. Ivchenko, X. Marie, T. Amand, K. Sakoda, G. Wang, and B. Urbaszek

Applied Physics Letters 105, 082111 (2014)

“Carrier and polarization dynamics in monolayer MoS₂”

D. Lagarde, L. Bouet, X. Marie, C.R. Zhu, B.L. Liu, P.H.Tan, T. Amand, B. Urbaszek

Physical Review Letters 112, 047401 (2014),

“Nuclear magnetization in gallium arsenide quantum dots at zero magnetic field”

G. Sallen, S. Kunz, T. Amand, L. Bouet, T. Kuroda, T. Mano, D. Paget, O. Krebs, X. Marie, K. Sakoda, B. Urbaszek*, **Nature Communications** 5, 3268 (2014)

“Nuclear spin physics in quantum dots: an optical investigation”

B. Urbaszek, X. Marie, T. Amand, O. Krebs, P. Voisin, P. Maletinsky, A. Högele and A. Imamoglu

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Spintronics based on magnetic tunnel junctions

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Magnetic tunnel junctions consist of two magnetic electrodes separated by very thin insulating barrier, which exhibits the large magnetoresistance effect originating from a quantum mechanical spin asymmetry of an electronic structure of a magnetic layer and/or interface. In early days of research the magnetoresistance ratio is below 20% [1-2]. Through the discovery of MgO crystalline barrier [3,4], the highest magnetoresistance ratio is over 600% at room temperature [5]. Nowadays, magnetic tunnel junctions are one of the core devices in various spintronics applications, in particular magnetic memory and sensors.

Here, I will talk our recent research on magnetic tunnel junctions utilizing various kinds of functional materials, e.g., magnetic tunnel junctions with hard magnets for high density magnetic random access memory applications [6,7], magnetic spin-valves with organic semiconductors [8,9]. Also, I would like to briefly mention possibilities to develop THz spintronics applications [10] and picotesla magnetic sensors for medical applications [11] using magnetic tunnel junctions.

These works were supported in part by Development of an infrastructure for normally-off computing technology project, ImPACT, S-Innovation project, and KAKENHI (Nano-Spin Conversion Science) in Japan.

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Publications

1. Q. L Ma, X. M. Zhang, T. Miyazaki, S. Mizukami, "Artificially engineered Heusler ferrimagnetic superlattice exhibiting perpendicular magnetic anisotropy", *Sci. Rep.* 5, 7863 (2015).
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Spin electronics sensors for biomagnetic signals detection and medical imaging

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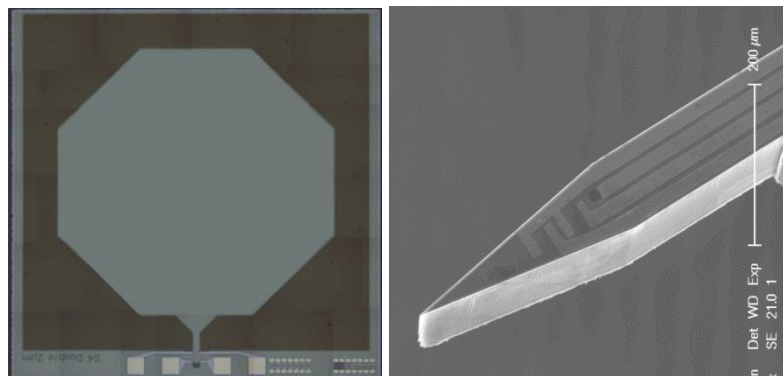
Spin electronics have opened the field of numerous applications in data storage, magnetic field sensing or MRAM. In particular, spin valve devices offer very good sensitivity – below the nanotesla range at room temperature - and since these systems are field sensors and not flux sensors, their sensitivity is weakly dependent with their size, and they can maintain very good performance at extremely small scale, allowing integration of multiple sensors or very small size magnetometer.

Magnetometry addresses many fields, from industrial, as in car industry, to more fundamental problems like in space-magnetometry or biomagnetism.

Biomagnetism, being defined by the very weak signature of magnetic fields generated by living tissues and organisms, either by magnetic particles embedded or attached to cells, or by the electrical activity such as neural currents, requires extremely sensitive sensors to reach the picotesla to femtotesla range of the corresponding signals. Superconducting Quantum Interference Devices (SQUIDS), operating at liquid helium temperature, have been the preferred type of sensors for this purpose.

We have developed new types of magnetometers based on spin electronics [1] to allow measuring the weak fields generated the electrical activity of heart, brain or neuron cells. These sensors exhibit field sensitivities ranging from the nanotesla (10^{-9}T) down to the femtotesla (10^{-15}T).

The principles of the sensors and their operation for magnetic cardiac mapping [2], low field Magnetic Resonance Imaging (MRI) [3], [4] or local neuronal electromagnetic activity will be shown in this contribution.



Left : Micrograph of a femtotesla-sensitivity magnetometer for Magneto-Cardiography and Low field MRI ; Right : Needle-shape Giant Magneto-Resistance sensor for local electromagnetic neuronal signal detection.

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Fields of Research

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Publications

1. *Noise in GMR and TMR sensors*, C. Fermon and M. Pannetier-Lecoœur, In *Giant Magnetoresistance (GMR) sensors, from Basis to State-of-the-Art applications*, Springer (2013), Editors: C. Reig, S. Cardoso de Freitas, S. C; Mukhopa.
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Surface Atomic-layer Superconductors on Silicon: Electron Transport, STM, and Control with Molecules

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Surface reconstructions of silicon and related semiconductors with metal adatoms constitute a family of highly-ordered low dimensional materials, which are fundamentally different from their bulk counterparts. In this talk, I report on the superconductivity of Si(111)-($\sqrt{7}\times\sqrt{3}$)-In surface revealed by lateral electron transport measurement and scanning tunneling microscopy (STM) studies [1-4]. The superconducting transition was evidenced by observations of the zero resistance state and I - V characteristics exhibiting sharp switching below 3 K. Superconducting vortices were observed by taking differential conductance (dI/dV) images using an STM at 0.5 K while magnetic field was applied. Vortices trapped along atomic steps exhibits characteristics of Josephson vortex, showing that an atomic step works as a Josephson junction (Fig. 1). Furthermore, we found that different kinds of phthalocyanine (Pc) molecules self-assembled on the Si(111)-($\sqrt{7}\times\sqrt{3}$)-In surface modified its superconductivity according to their magnetic properties. This clearly shows the possibility of controlling the macroscopic superconducting properties of surface reconstructions utilizing its surface sensitivity.

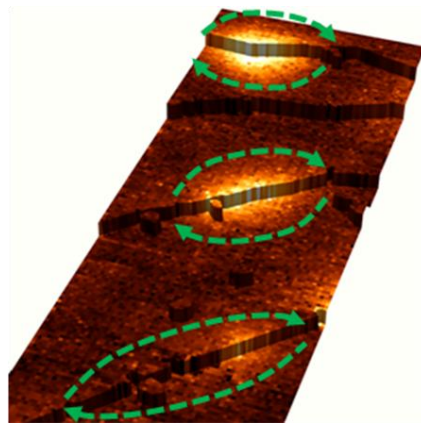


Fig.1 3D representation of vortices trapped along the atomic steps of a Si(111)-($\sqrt{7}\times\sqrt{3}$)-In surface. The color scale indicates the zero bias conductance measured using STM while the height topographic height.

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- [2] T. Uchihashi et al., Nanoscale Res. Lett. **8**, 167 (2013).
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Education

1995 Ph.D. in Science from the University of Tokyo

Professional Experience

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2003-2008 Researcher, Nanoscale Quantum Conductor Array Project, ICORP, JST

2004 - Present Senior researcher (MANA Scientist), National Institute for Materials Science, Japan

2006 Visiting researcher, Institute of Experimental and Applied Physics, Christian-Albrechts-Universität zu Kiel, Germany

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Fields of Research

Surface Science, Nanomaterials, Low-temperature Physics

Publications

1. S. Yoshizawa, H. Kim, T. Kawakami, Y. Nagai, T. Nakayama, X. Hu, Y. Hasegawa, and T. Uchihashi, Phys. Rev. Lett. **113**, 247004(1-5) (2014). [Editors' Suggestion and Featured in *Physics*]
2. T. Uchihashi, P. Mishra, and T. Nakayama, Nanoscale Res. Lett. **8**, 167(1-7) (2013).
3. T. Uchihashi, P. Mishra, M. Aono, and T. Nakayama, Phys. Rev. Lett. **107**, 207001(1-4) (2011). [Editors' Suggestion and Featured in *Physics*]
4. T. Uchihashi, C. Ohbuchi, S. Tsukamoto, and T. Nakayama, Phys. Rev. Lett. **96**, 136104(1-4) (2006).
5. T. Uchihashi and U. Ramsperger, Appl. Phys. Lett, **80**, 4169-4171 (2002).

Coherence in spin chain: a new route for quantum computation and communication.

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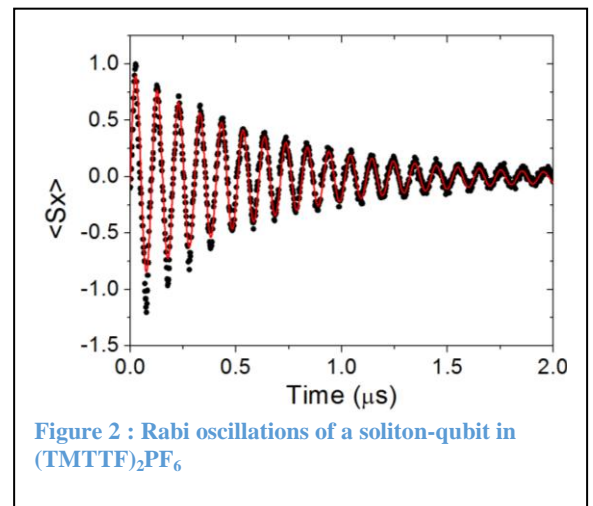
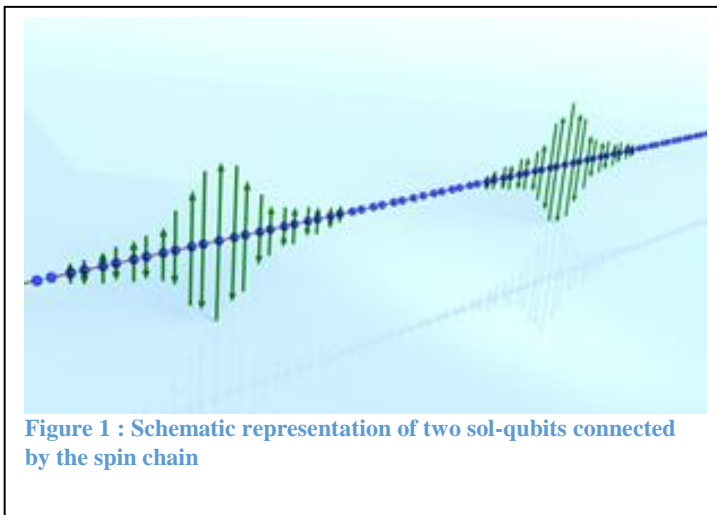
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Coherence of electron spin has attracted a great interest for the last decade due to its potential application as quantum bits i.e. elementary piece of a quantum computer. Usually, electron spin qubits are made of paramagnetic impurities [1,2], which lose their coherence because of the environment interactions (spin bath, phonon bath...).

Hereby we will present a completely new concept: in strongly correlated Heisenberg spin chain, the isotropic exchange protects the loss of quantum memory. A non magnetic defect polarizes the surrounding spins and creates a quantum soliton of total spin $S=1/2$. Since the soliton belongs to the chain it is protected from the environment by the exchange interaction. Moreover, it has been proved theoretically that two qubits belonging to the same spin chain are by nature entangled (necessary condition for quantum communication). However, up to now, no observation of quantum coherence in such a system has been reported.

We will show the first observation of quantum coherence in electron spin solitons in the organic chain $(\text{TMTTF})_2\text{PF}_6$ [3]. This result paves the way for the implementation of a different type of quantum computer.



[1] Bertaina S. et al. *Nature Nanotechnology* **2**, 39 - 42 (2007)

[2] Bertaina S. et al. *Nature* **453**, 203-208 (2008)

[3] Bertaina S. et al. *Phys. Rev. B* **90** 060404 (2014)

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Fields of Research

Electron spin qubit, electron paramagnetic resonance, magnetism, strongly
correlated electron

Publications

1. Shim J., Bertaina S., et al., *Physical Review Letters* **109**, 050401 (2012).
2. Bertaina S., et al. *Physical Review Letters* **103**, 226402 (2009)
3. Bertaina S., et al. *Physical Review Letters* **102**, 050501 (2009)
4. Bertaina S., et al. *Nature* **453**, 203-208 (2008)
5. Bertaina S., et al. *Nature Nanotechnology* **2**, 39 - 42 (2007)

Predicting new carbon nanomaterials from first principles

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Atomic scale computer modelling can be used in various ways in the field of nanomaterials science. Its role has traditionally been to support experimental work: for example discriminating between different structural models based on agreement of simulated spectra with available experimental data. Recent advances in both computer power and available algorithms mean we now have an unprecedented level of accuracy with atomic simulations, and the capability of routinely modelling extremely large scale systems containing many thousands of atoms. This allows us to move beyond confirmation of experimental findings towards realistic predictive models.

In this talk I will present some of our recent work using DFT calculations to help develop new “virtual materials”, such as two-dimensional networks of extended pi-conjugated polymers, edge control in carbon nanoribbons, and new approaches to indirect chemical doping in carbon nanotubes [1]. I will highlight ongoing collaborations with Japanese institutions, notably a new double degree programme with Toyo University [4], and links with Nagoya University (including an EU IRSES project on fluorinated nanocarbons [5]).

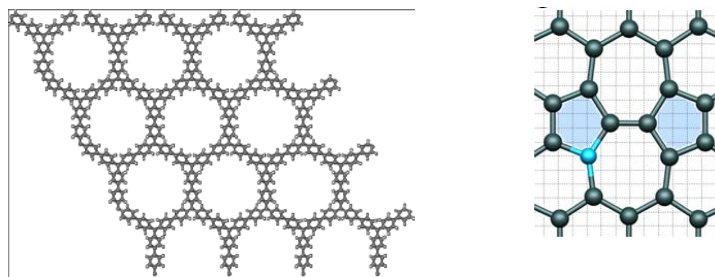


Figure: (left) 2D-network of conjugated polymers [2], (right) Substitutional nitrogen impurity in graphene, neighbouring a structural defect (5-7-7-5 “Stone-Thrower-Wales” defect) [3]

- [1] All publications available from www.ewels.info
- [2] *Dirac Cones in two-dimensional conjugated polymer networks*, J.-J. Adjizian, P. Briddon, B. Humbert, J.-L. Duvail, Ph. Wagner, C. Adda, C. Ewels, **Nat. Commun.** 5, 5842 (2014)
- [3] *Atomic Configuration of Nitrogen-Doped Single-Walled Carbon Nanotubes*, R. Arenal, K. March, C. Ewels, X. Rocquefelte, M. Kociak, A. Loiseau, O. Stephan, **Nano Letters**, 14, 5509 (2014)
- [4] <http://www.toyo.ac.jp/site/bionano/39003.html>
- [5] <http://www.nanocf.eu/index.php?id=2748&type=0&L=0>

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In close collaboration with experimental colleagues, I use atomic scale computer simulations to understand and design new carbon-based nanostructures with unique customised properties, either through new structural topologies or chemical and structural modification.

Refereed Publications	123	Total Publications	133
Book Chapters	6	H-index	29

Responsibilities

Coordinator Nanocarbon Transversal Action at the Institute (22 full-time researchers)

Coordinator, EU Marie Curie Training Network “Enabling Excellence” (2015-2019)

Visiting Researcher, Bio-Nano Electronics Centre, Toyo University, Tokyo, Japan (2013-2018)

Trustee (director) for the Vega Science Trust, Science Communication Charity www.vega.org.uk

Committee Member British Carbon Group (2002-), GDRI-GNT (Graphene-Nanotubes) (2008-)

Editorial advisory board, “Materials Today” (2011)

Conference co-organiser annual “NanoteC” international series (1998-2010)

Reviewer for Phys Rev, ACS, ..., regular project review for EU, PRACE, ANR (France), NSF, FNRS, ...

Previously

2003-2005 Marie Curie Individual Fellowship, Université Paris Sud, Orsay, (Christian Colliex)

2002-2003 TMR Postdoc, Composite Materials, ONERA, Paris, (Annick Loiseau)

1997-2002 2 days/week: Dept. Chemistry, Sussex University, UK (Malcolm Heggie)

1999-2002 3 days/week: The Vega Science Trust (Harry Kroto)

Charity communicating science in the media. Developed Europe’s first science TV channel broadcast over Internet. Researched programmes, production public relations.

1993-1997 PhD « Research Assistant », Physics Department, Exeter University (Bob Jones)

1989-1993 Degree BA(Hons) 2:1, Metallurgy and Materials, Keble College, Oxford University

Prizes, distinctions

- 7th British Carbon Group ‘Ubbelohde Award Lecture’ for Carbon Science (2014)
- EU Marie Curie Excellence Award (2006)

Chris Ewels graduated from Oxford University in 1993 after studying “Metallurgy and the Science of Materials”, with a fourth year at the Max Planck Institute for Powder Metallurgy. He received a Ph.D. in 1997 from the University of Exeter UK, for computational studies of oxygen defects in silicon. He then moved to Sussex University where he worked on radiation induced defects in graphite and carbon nanosystems. At Sussex he joined the Vega Science Trust with Sir Harry Kroto, where he created an online science TV channel and developed a passion for public communication of science. In Paris he worked at ONERA and was then a Marie Curie Individual Research Fellow at the Université Paris Sud within the electron microscopy group of Professor Christian Colliex. In 2006 he took up a permanent post with the CNRS at the Institute of Materials in Nantes.

His work focuses on computer modelling of point and line defects in nanoscale carbons and oxides, and he has authored over 100 journal publications including six book chapters. His interest in science communication continues, having exhibited his nanoscience art in the US (www.ewels.info) and established an award winning EU funded nanoscience web video project (www.youtube.com/nano2hybrids). In 2006 he received the European Marie Curie Excellence Award. He now runs the transversal nanocarbon action at the Institute of Materials in Nantes. His links with Japan began with a 2 month visit in 2006 to the Electron Microscopy Group of Prof. Kazu Suenaga at AIST Tsukuba. Since then he travels regularly to Japan. With Prof. Toru Maekawa he has established the first ‘double degree programme’ for exchange of PhD students between Nantes University and Toyo University’s BioNano Centre. He also collaborates with the fullerene research group of Prof. Shinohara at Nagoya, and is involved in a European network “NanoCF” with Stephen Irle at Nagoya University exploring fluorinated nanocarbon materials.

Chemical bonding networks and their role on the structure of complex metallic alloy surfaces

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Complex Metallic Alloys (CMAs), intermetallic compounds made of at least two elements, have a crystalline structure that differs from usual alloys by the number of atoms in their unit cell and the occurrence of highly symmetric clusters as alternative structural unit [1]. Recently, quantum chemical calculations performed on several types of Al-TM (TM=Cu, Co, Fe...) CMAs have highlighted the existence of specific covalent interactions within the bulk [2,3]. In the case of the Al₁₃TM₄ systems, this has led to a better understanding of their physical properties and to a description of their structure as 3-D cage compounds [3]. While well identified in the bulk materials, questions arise on how these chemical bonding networks will affect the atomic structure of CMA surfaces.

Here, we will present recent structural investigations of complex Al-TM surfaces using both experimental and *ab initio* computational methods [4,5]. It will be demonstrated that the surface terminations can be associated to planes present in the bulk crystal structure. For several phases, these planes remain incomplete when exposed at the surface. We will show how this reduced atomic density can be related to the presence of chemical bonding network in the materials.

Finally, among the systems studied, some of them have been recently considered as promising candidates for the heterogeneous hydrogenation catalysis [6]. We will discuss how their atypical surface structure and associated atomic ensembles could explain the catalytic properties reported in line with the site-isolation concept [7].

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[4] J. Ledieu, et al., *Phys. Rev. Lett.* **110**, 076102(2013).

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[6] M. Armbrüster, et al., *Nature Materials* **11**, 690 (2012).

[7] K. Kovnir, et al., *Science and Technology of Advanced Materials* **8**, 420 (2007).

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Education

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2001 - PhD in Surface Science, The University of Liverpool, UK.
1997 - BsC with "Hons" in Applied Physics, The University of Central Lancashire, UK.

Professional Experience

2009- CNRS Research Scientist at the IJL UMR 7198, Nancy, France.
2005-2008 CNRS Research Scientist at the LSG2M UMR 7584, Nancy, France.
2000-2004 Post-doctorate position at the SSRC, The University of Liverpool, UK.

Fields of Research

Surface, complex metallic alloys, thin films, quasicrystal

Publications

1. M. Meier, J. Ledieu, M.-C. De Weerd, Ying-Tzu Huang, G. J. P. Abreu, K. Pussi, R. D. Diehl, T. Mazet, V. Fournée, and É. Gaudry, *Phys. Rev. B* **91**, 085414 (2015)
2. J. Ledieu, É. Gaudry and V. Fournée, *Sci. Technol. Adv. Mater.* **15**, 034802 (2014).
3. V. Fournée, É. Gaudry, J. Ledieu, M.-C de Weerd, D. Wu and T. Lograsso, *ACS Nano* **8**, 3646 (2014).
4. J. Ledieu, É. Gaudry, L. N. SerkovicLoli, S. AlarcónVillaseca, M.-C. de Weerd, M. Hahne, P. Gille, Y. Grin, J.-M. Dubois and V. Fournée, *Phys. Rev. Lett.* **110**, 076102 (2013).
5. L.N. SerkovicLoli, É. Gaudry, V. Fournée, M.-C. de Weerd and J. Ledieu, *Phys. Rev. Lett.* **108**, 146101 (2012).

Diffusion driven layer-by-layer assembly of nanosheets into porous three-dimensional structure

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One of the critical challenges for the practical application of graphene and its derivatives is developing a robust and versatile assembly method which allows the construction of the nanosheets into functional macroscopic structures appropriate for integration with conventional real-life devices. To address this issue, we utilize the fact that graphene oxide is that they often behave as charged macromolecules, and thus can readily interact with an oppositely charged polyelectrolyte to form a stable complex. In this report, we demonstrate how such complexation process could be utilized for directing the self-assembly of nanosheets. Herein, we introduce a novel “diffusion driven layer-by-layer” assembly and demonstrate its application for the construction of graphene oxide (GO) sheets into porous three-dimensional structures. The process utilizes the interaction of GO with branched polyethylenimine (b-PEI), a positively charged polyelectrolyte, to form a stable complex. Interestingly, when this reaction is confined at a liquid/liquid interface, we observe that the diffusion of b-PEI allows the GO/b-PEI complex formed at the interface to continuously grow into a foam-like framework which porosity can be tuned from ultra-light (5.6 mg/cm^3) to tightly packed ($\sim 1700 \text{ mg/cm}^3$) through simple adjustments. Furthermore, the assembly process can be utilized in various configurations such as to create free-standing architectures with tailored shapes or patterned films on a substrate. The obtained GO structures are quite stable and can be reduced using various methods. This novel assembly method opens pathway to many useful nanosheet superstructures, and may be further extended to other types of nanomaterials in general.

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Education

- 1999~2005 UC Berkeley, Ph. D. in Chemistry
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Dissertation title: *“Toward metal nanoarchitectonics: shape-controlled synthesis and assembly of metal nanoparticles”*
- 1996~1999 Seoul National University, B. S. in Chemistry

Professional Experience

- 2011~ Kyoto University, Institute for Integrated Cell-Material Sciences (iCeMS)
iCeMS Kyoto Fellow / Independent assistant professor
- 2007~2010 Northwestern University, Dept. of Materials Science and Engineering
Postdoctoral research, Advisor: Prof. Jiaying Huang
- 2005~2007 UC Berkeley, Dept. of Bioengineering
Postdoctoral research, Advisor: Prof. Luke P. Lee
- 1999~2005 UC Berkeley, Dept. of Chemistry
Ph. D. research, Advisor: Prof. Peidong Yang
- 1998~1999 Seoul National University, Dept. of Chemistry
Undergraduate research, Advisor: Prof. Jin Ho Choy

Fields of Research

Self-assembly, nanomaterials

Publications

1. J. Zou, F. Kim, *Nat. Commun.* (2014) DOI: 10.1038/ncomms6254
2. J. Zou, F. Kim, *ACS Nano*, **6**, 10606 (2012)

Hydrogen-Induced Fracture: From Fundamentals to Prognosis

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Development and validation of a lifetime prediction methodology for failure of materials used for hydrogen containment components are of paramount importance to the planned hydrogen economy. In this presentation, we summarize recent developments on fracture prognosis for various materials by accounting for the deformation mechanisms at the microscale.

Recent experimental studies of the microstructure beneath fracture surfaces of ferritic steel, lath martensitic steel, stainless steel and nickel specimens fractured in hydrogen suggest that the dislocation structure and hydrogen transported by mobile dislocations play important roles in the evolution of the fracture process/event. After reviewing this plasticity-mediated hydrogen-induced failure, we present a revised model for hydrogen/deformation interactions in order to account for dislocation transport along with stress driven diffusion and trapping at microstructural defects.

Arguably the most devastating mode of hydrogen-induced degradation is the hydrogen embrittlement of high-strength steels which results in a sharp transition from a high-toughness ductile (microvoid coalescence) fracture to a low-toughness brittle intergranular fracture. We present an approach to quantify this effect of hydrogen on the fracture resistance of a low alloy martensitic steel through the use of a statistically-based micromechanical model for the critical local fracture event which relates the influence of hydrogen adsorbed at internal interfaces in affecting decohesion to the onset of macroscopic failure.

Lastly, we present an approach to mitigate the hydrogen effect on ferritic systems subjected to cyclic loading. Based on experiments, materials physics, and applied mechanics methodology, we have recently found and quantified that a few molecules of oxygen per million molecules of hydrogen can markedly increase the magnitude of the stress intensity factor range at which hydrogen-accelerated fatigue commences.

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Education

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Professional Experience

Assistant Professor, Department of Theoretical and Applied Mechanics, University of Illinois at Urbana-Champaign, 1991-1997
Associate Professor, Department of Theoretical and Applied Mechanics, University of Illinois at Urbana-Champaign, 1997-2004
Professor, Department of Mechanical Science and Engineering, University of Illinois at Urbana-Champaign, 2004-present
Director, International Institute for Carbon-Neutral Energy Research (I2CNER), Kyushu University, Japan, 2010-present

Fields of Research

Environmental degradation of materials, solid mechanics, finite element methods.

Publications

1. Dadfarnia, M., Martin, M. L., Nagao, A., Sofronis, P. and Robertson, I. M., *J. Mech. Phys. Solids*, In Print.
2. Nagao, A., Martin, M. L., Dadfarnia, M., Sofronis, P. and Robertson, I. M., *Acta Materialia*, **74**, 244 (2014).
3. Somerday, B. P., Sofronis, P., Nibur, K. A., San Marchi, C. and Kirchheim, R. *Acta Materialia*, **61**, 6153 (2013).
4. Martin, M. L., Somerday, B. P., Ritchie, R. O., Sofronis, P., Robertson, I. M., *Acta Materialia*, **60**, 2739 (2012).
5. Novak, P., Yuan, R., Somerday, B., Sofronis, P. and Ritchie, R. O., *J. Mech. Phys. Solids*, **58**, 206 (2010)

Mixed anion compounds with functional properties

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Mixed anion compounds such as oxychlorides, oxychalcogenides, oxyhydrides and oxynitrides are an emerging class of materials with intriguing properties, including solar-activated photocatalyst BaTaO_2N , high-temperature superconducting iron pnictides, EuNbO_2N with colossal magnetoresistance, spin liquid system $(\text{CuCl})\text{LaNb}_2\text{O}_7$ and transparent p-type semiconducting system LaCuOS , to name only a few.

My talk will mostly focus on the synthesis, structure and properties of several transition-metal oxyhydrides. $\text{ATi}(\text{O},\text{H})_3$ (A = alkali metal) can be obtained in a topochemical fashion using CaH_2 reduction of the corresponding oxide hosts [1]. $\text{ATi}(\text{O},\text{H})_3$ is metallic with high carrier concentrations, though it fails to be superconducting at least down to 0.5 K [2]. Besides, hydride (H^-) ions are quite mobile at moderate temperatures, implying potentials of the oxyhydrides as ionic conductors and catalysts. Multistep reactions via oxyhydride will also be shown.

Mixed anion perovskite-based structures such as SrCrO_2H and MnTaO_2N can be prepared by high temperature and high pressure reaction [3, 4]. For SrCrO_2H , despite the non-bonding nature in Cr 3d and H 1s orbitals, the magnetic order temperature is as high as 380 K, which is significantly higher than those in isoelectric (Cr^{3+}, d^3) with LnCrO_3 (Ln = rare earth). This can be reasonably explained by octahedral tilting scheme.

We have prepared new titanium oxypnictides $\text{BaTi}_2\text{Sb}_2\text{O}$ and $\text{BaTi}_2\text{Bi}_2\text{O}$. A novel electronic phase diagram has been found in the solid solution $\text{BaTi}_2(\text{Sb},\text{Bi})_2\text{O}$, where two superconducting phases are separated by a metallic phase [5]. Similar phase diagram is also seen in high- T_c superconducting iron arsenides.

[1] Y. Kobayashi et al., *Nat. Mater.* **11**, 507 (2012).

[2] T. Yajima et al., *J. Am. Chem. Soc.* **134**, 8782 (2012).

[3] C. Tassel et al., *Angew. Chem. Int. Ed.* **53**, 10377 (2014).

[4] C. Tassel et al., *Angew. Chem. Int. Ed.* **54**, 516 (2015).

[5] T. Yajima et al., *J. Phys. Soc. Jpn.* **82**, 033705 (2013).

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Education

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Professional Experience

Assistant Professor, Institute for Solid State Physics, University of Tokyo, 1998-2003
Associate Professor, Department of Chemistry, Graduate School of Science, Kyoto University, 2003-2009
Professor, Department of Hydrocarbon Chemistry, Graduate School of Engineering, Kyoto University, 2010-present

Fields of Research

Solid State Chemistry, Solid State Physics

Publications

1. Kageyama H. et al., *Phys. Rev. Lett.* **82**, 3168 (1999).
2. Tsujimoto Y. et al., *Nature* **450**, 1062 (2007).
3. Kawakami T. et al., *Nat. Chem.* **1**, 371 (2009).
4. Kobayashi Y. et al., *Nat. Mater.* **11**, 507 (2012).
5. Frandsen B. et al., *Nat. Commun.* **5**, 5761 (2014).

New solid adsorbents for metals recovery from liquid wastes

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The current explosive development of high tech devices (communication devices, light emitters, magnetic materials, sensors, hardwares ...) relies on a handful of so-called “strategic metals”, whose specific properties makes them essential.

Unfortunately, most of them are rare and/or quite diluted in the earth crust. This limits their supply, with huge consequences in terms of availability and costs.

The recovery of these strategic metals from recycled sources thus appears more and more as an essential component of the future supply chains.

Within this frame we developed a new generation of solid adsorbents, allowing for the very selective recovery of targeted metals from various liquid solutions. Some of our results will be presented and discussed.

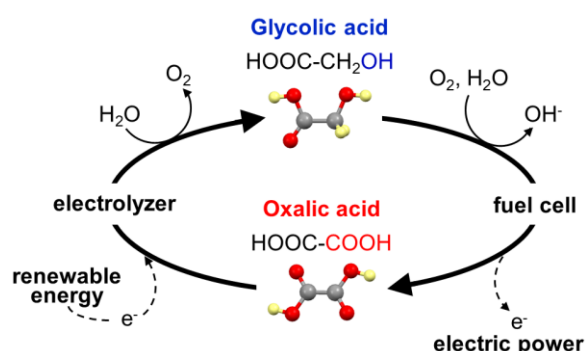
Direct electric power charge and discharge without CO₂ emission using an alcohol/carboxylic acid redox couple

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An excessive increase of CO₂ in the atmosphere is regarded as the most probable cause of global warming. A substantive transition from fossil-based systems to systems operated by electricity that is generated using renewable energy, i.e., “renewable electricity”, seems to be the optimal answer to this environmental issue. A lack of efficient distribution techniques for unstably supplied and unevenly distributed renewable electricity is one of the fundamental impediments to its practical use. Thus, electric power storage in high-energy chemicals, called “energy carriers”, has received much attention for the efficient storage and on-demand supply of renewable electricity.¹ Here, we demonstrate an electric power circulation method that does not emit CO₂ and is based on the glycolic acid (GC)/oxalic acid (OX) redox couple (Scheme 1).² Direct electric power storage in GC ensures considerable high energy density storage and good transportability through OX electroreduction with significantly high selectivity (>98%) using pure anatase-type titania (TiO₂) spheres under mild conditions in the potential region of -0.5 to -0.7 V vs. the RHE at 50 °C (Figure 1). The most desirable characteristic of this electroreduction is the suppression of hydrogen evolution even in acidic aqueous media (Faraday efficiency of 70–95%, pH 2.1). We also successfully generated power without CO₂ emissions via selective electrooxidation of GC with an alkaline fuel cell.



Scheme 1 Carbon-neutral energy cycling using the GC/OX redox couple. Grey, red and yellow spheres represent carbon, oxygen and hydrogen atoms, respectively.

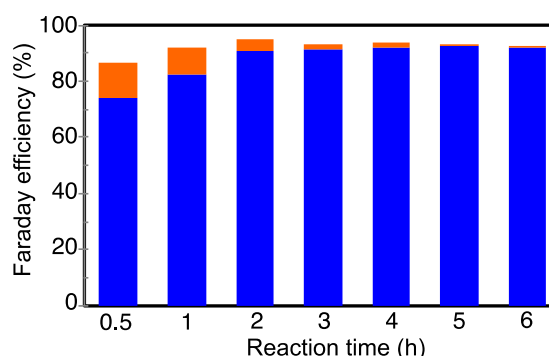


Figure 1. Faraday efficiencies for the formation of GC (blue) and glyoxalic acid (orange) at -0.7 V vs. RHE and 50 °C.

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[2] R. Watanabe, M. Yamauchi, M. Sadakiyo, R. Abe, T. Takeguchi, *Energy & Environmental Science*, in press

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Education

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Assistant Professor, Department of Chemistry, Kyushu University, 2003-2008
Associate Professor, Catalysis Research Center, Hokkaido University, 2008-2011
Associate Professor, International Institute for Carbon-Neutral Energy Research, Kyushu University, 2012-

Fields of Research

energy-related chemistry, solid state chemistry, nanomaterials, catalysis, hydrogen-related chemistry

Publications

1. T. Matsumoto, M. Sadakiyo, M. L. Ooi, T. Yamamoto, S. Matsumura, K. Kato, T. Takeguchi, N. Ozawa, M. Kubo, M. Yamauchi, *Physical Chemistry Chemical Physics*, in press
2. R. Watanabe, M. Yamauchi, M. Sadakiyo, R. Abe, T. Takeguchi, *Energy & Environmental Science*, in press
3. T. Matsumoto, M. Sadakiyo, M. L. Ooi, S. Kitano, T. Yamamoto, S. Matsumura, K. Kato, T. Takeguchi, M. Yamauchi, *Scientific Report*, **4**, 5620 (2014)
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Phase transitions at the nanoscale: development of thermoporosimetry as a multi-scale tool for the characterization of complex materials

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Porous materials are omnipresent in nature and find various industrial applications. Numerous biological processes also involve such porous materials making them the object of abundant studies. The characterization of porosity is therefore a crucial issue.

Gas sorption and mercury intrusion porosimetry are probably the most popular techniques. Thermoporosimetry (TPM) has also been proposed as an alternative^{1,2}. TPM relies on the Gibbs-Thomson equation which relates the shift of the transition temperature of a confined liquid ΔT to the radius of the pore in which it is confined.

This technique is particularly attractive because it offers the possibility to characterize porosity from the mesopore range up to the macroporous domain within a single experiment. It is also very unique because it allows the characterization of inorganic materials but also polymers and hybrids.

We will present recent developments of the technique in particular the first true calibration of TPM within the macropore range by using hierarchically porous hybrid materials³.

Several examples will be taken illustrating the potential of TPM for the characterization of complex materials processed by sol-gel chemistry.

The chosen examples will cover a wide range of applications from biomaterials⁴ to environmental remediation and catalysis.

[1] New calorimetric approaches to the study of soft matter 3D organization

J.M. Nedelec and M. Baba, *Tomorrow's Chemistry Today: Concepts in Nanoscience, Organic Materials and Environmental Chemistry*, Ed. B. Pignataro, Wiley-VCH Weinheim, (2008) 237-258.

[2] J.M. Nedelec, J.P.E. Grolier and M. Baba, *J. Sol-Gel Sci. Technology*, **40**, (2006) 191-200.

[3] A. Hardy Dessources, S. Hartmann, M. Baba, N. Huesing and J.M. Nedelec, *J. Mat. Chem.* **22** (2012) 2716-2720

[4] J. Soulié, A. Hardy-Dessources, J.-M. Nedelec, E. Jallot, *J. Phys. Chem. C* **117**(13), (2013), 6702-6711

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Education

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Professional Experience

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1999 : Assistant Professor (MCF) at Ecole Nationale Supérieure de Chimie de Clermont-Ferrand

2010 : Professor at ENSCCF

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Fields of Research

Sol-gel chemistry; soft chemistry; Porous materials; Bioceramics; Confinement effect in materials

Recent Publications

New calorimetric approaches to the study of soft matter 3D organization

J.M. Nedelec and M. Baba, Tomorrow's Chemistry Today: Concepts in Nanoscience, Organic Materials and Environmental Chemistry, Ed. B. Pignataro, Wiley-VCH Weinheim, (2008) 237-258.

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A. Lukowiak, J. Lao, J. Lacroix, J.-M. Nedelec, Chem. Commun., 49, (2013), 6620-6622

In situ property measurement of inorganic nanomaterials under TEM

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Understanding the mechanical properties of inorganic nanomaterials is not only fundamentally interesting but also practically important, because of their broad applications, ranging from energy storage to composite materials, where the mechanical properties will determine the structural reliability and long-time performance. In situ transmission electron microscopy (TEM) is unique for probing mechanical properties at nanometer scale, simultaneously enabling manipulation at sub-nanometer precision, quantitative mechanical measurement with nanonewton accuracy, and deformation mechanisms at atomic resolution.

In my talk, I will present our recent works on the mechanical properties of inorganic nanomaterials by applying the in situ TEM method.(1) In addition to the intrinsic chemical bonding and famous size effects, we investigated the influences of the “microstructures” and external loading conditions. Due to an interlocked joint geometry, the deformation mechanism of bamboo-shaped BNNTs was switched from an interplanar sliding mode to an in-plane tensile elongation mode, with tensile strength up to 8.0 GPa.(2) Due to the different stress states, Si nanowires showed distinct deformation behaviors under tension and bending. Under tension, Si NWs deformed elastically until brittle fracture. Under bending, the Si NWs demonstrated considerable plasticity, with a crystalline-to-amorphous phase transition.(3) Due to the surface energy, the bending behaviors of MoS₂ atomic layers demonstrated strong size dependence, from spontaneous rippling (<5 atomic layers) to homogeneous curving (~10 layers) and to kinking (>20 layers).(4) Our work has greatly enriched the understanding of mechanical properties of inorganic nanomaterials and offers valuable guidelines for the design of mechanically reliable nanodevices.

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2. Tang D-M, Ren C-L, Wei X, Wang M-S, Liu C, Bando Y, & Golberg D (2011) Mechanical Properties of Bamboo-like Boron Nitride Nanotubes by In Situ TEM and MD Simulations: Strengthening Effect of Interlocked Joint Interfaces. *ACS Nano* 5(9):7362-7368.
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1996 Supervising Researchers, Advanced Beam Analysis Station, NIRIM
2001 Director of the Integrated Strategy Office at National Institute of Materials Science (NIMS)
2003 Director-General, International Center for Young Scientists (ICYS), NIMS
2004 NIMS Fellow
2007 Chief Operating Officer (COO), MANA, NIMS
2008 Visiting Professor, Waseda University

Fields of Research

He has been working on “Synthesis and property measurements of novel 1D/2D nanomaterials such as BN nanotubes and nanosheets”. He has succeeded in producing high purity and large scale BN nanotubes. He has received a number of awards including the 3rd Thomson Reuters Research Front Award (2012) and the 16th Tsukuba Prize (2005). He has been selected as ISI Highly Cited Researchers in Materials Science (2014). He is now an adjunct member of the Science Council of Japan and also a Fellow of The American Ceramic Society.

Selected Recent Publications:

1. Zhi, C., Xu, Y., Bando, Y. and Golberg, D., *ACS Nano*, 5, 6571-6577 (2011)
2. Wang, X., Zhi, C., Li, L., Zeng, H., Li, C., Mitome, M., Golberg, D. and Bando, Y., *Adv. Mater.*, 23, 4072-4076 (2011)
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In situ compression in Transmission Electron Microscopy and mechanical analysis of ceramic nanoparticles

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Nanometer-sized objects are attracting large attention nowadays due to their amazing mechanical properties in comparison to their bulk counterparts. In particular, they can exhibit far larger and size-dependent elastic limits [1]. Several mechanisms have been proposed, among which dislocation nucleation at the surfaces.

Large numbers of studies are nowadays dedicated on plastic deformation of metals at the nano-scale. On ceramic materials, the works from Korte et al. [2] on MgO, or Calvié et al. [3] on transition alumina nanoparticles showed that these materials can exhibit significant plastic deformation, whereas the corresponding bulk materials are brittle. A better comprehension of the mechanisms involved in the deformation of ceramics at the nanoscale could help optimizing their fabrication process.

The mechanical properties of ceramic nano-objects of a few tens of nanometer can be studied using in situ compression tests in TEM. This technique will be applied on MgO nanocubes. Firstly, deformation mechanisms will be proposed from the contrasts in the images and Molecular Dynamics simulations [4]. Secondly, a mechanical behavior law will be identified from the images and the force-displacement curves through Digital Image Correlation and Finite Elements Simulations. The parameters (Young modulus, yield stress) will be discussed in function of the observation conditions as well as the nanocube size, to study a possible size effect.

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Professional Experience

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Associate professor, Nancy I University, France, 2000-2002.

Associate professor, INSA-Lyon, France, 2002-2007

Professor, INSA-Lyon, France, 2007-...

Fields of Research

Electron microscopy (SEM, TEM), *in situ*, environmental, tomography

Publications

1. Issa I, Amodeo J, Réthoré J, Joly-Pottuz L, Esnouf C, Morthomas J, Perez M, Chevalier J; Masenelli-Varlot K, *Acta Materialia*, **86**, 295-304 (2015)
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Atomic-scale investigation of surfaces/interfaces of energy materials

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Transition-metal oxides show a variety of phenomena at their surfaces and interfaces, which have been induced by structural and electronic modifications. Although recent technical advances in the synthesis of oxide thin films and heterostructures have provided a fertile new ground for creating those novel states at their surfaces and interfaces, the origins of the functionalities, on an atomic scale spatial resolution, remain far from understood.

In order to clarify the origins of such phenomena and to further explore intriguing functionalities, it is important to elucidate their electronic structures at the atomic level.

In this presentation, I discuss following points based on the observations using a scanning tunneling microscopy/spectroscopy (STM/STS) combined with pulsed laser deposition (PLD).[1]

1. Atomic structure of oxide substrate: SrTiO₃(100) [2]
2. Preparation of atomically-defined oxide substrate surface:
SrTiO₃(001)-($\sqrt{13} \times \sqrt{13}$)-R33.7° reconstructed surface [3, 4]
3. Growth processes of oxides:
SrTiO₃ [5], SrO [6], LaAlO₃, (LaCa)MnO₃, and SrVO₃
4. 2D TiO₂-nanomesh formation on LaAlO₃.

These STM/STS studies provide us of profound insights into the intriguing phenomena at oxide surfaces. Further, we aim to correlate our microscopic observation with macroscopic properties of oxides. Consequently, these findings on the atomic-scale nature are discussed with electron transport properties and magnetic properties of oxide thin films.

Further, If time allows, I would like to report the surprisingly low electrolyte/electrode (LiCoO₂) interface resistance of 8.6 Ω cm² observed in lithium thin-film batteries. This value is an order of magnitude smaller than that presented in previous reports on all-solid-state lithium batteries. The value is also smaller than that found in a liquid electrolyte based batteries. The low interface resistance indicates that the negative space-charge layer effects at the Li₃PO_{4-x}N_x/LiCoO₂ interface are negligible, and demonstrates that it is possible to fabricate all-solid state batteries with faster charging/discharging properties.

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Education

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Fields of Research

Solid State Chemistry, Solid State Physics, Surface Science

Publications

1. Ryota Shimizu, Katsuaki Sugawara, Kohei Kanetani, Katsuya Iwaya, Takafumi Sato, Takashi Takahashi, and Taro Hitosugi
“Charge-Density Wave in Ca-Intercalated Bilayer Graphene Induced by Commensurate Lattice Matching”
Phys. Rev. Lett. 114, 146103 (2015).
2. Masakazu Haruta, Susumu Shiraki, Tohru Suzuki, Akichika Kumatani, Takeo Ohsawa, Yoshitaka Takagi, Ryota Shimizu, and Taro Hitosugi
“Negligible “negative space-charge layer effects” at oxide-electrolyte/electrode interfaces of thin-film batteries”
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3. Ikutaro Hamada, Ryota Shimizu, Takeo Ohsawa, Katsuya Iwaya, Tomihiro Hashizume, Masaru Tsukada, Kazuto Akagi, and Taro Hitosugi
“Imaging the evolution of d-states at a strontium titanate surface”
J. Am. Chem. Soc. 136, 17201–17206 (2014).
4. Patrick Han, Kazuto Akagi, Filippo Federici Canova, Hiroataka Mutoh, Susumu Shiraki, Katsuya Iwaya, Paul S. Weiss, Naoki Asao, and Taro Hitosugi
“Bottom-Up Graphene-Nanoribbon Fabrication Reveals Chiral Edges and Enantioselectivity”
ACS Nano 8, 9181–9187 (2014).
5. Takeo Ohsawa, Ryota Shimizu, Katsuya Iwaya, Taro Hitosugi
“Visualizing atomistic formation process of SrO_x thin films on SrTiO₃”
ACS Nano 8, 2223–2229 (2014).

Nano and Meso- Control to Advance Polymeric Materials for Membrane Separation

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The Sivaniah group manipulates materials with synthetic and biological approaches whilst seeking to establish a viable interface between the two.

One example is the controlled generation of spatially variant stiffness in 2D gels to interrogate cell mechanotaxis (*Adv. Mater.* 2012). Moreover our group studies the generation of bioplastics using bacterial and enzymatic tools (*Adv. Mater.*, 2013). Through such works, we will develop practical principles that can support our vision of generating industrially relevant processes via bionanotechnology.

Although soft-matter bionanotechnology forms one key part of our research, we mix both synthetic and biosynthetic materials development (with a current focus in achieving energy efficiency and environmental targets in separation technology). Examples include a transformative platform technology for generating nanoporous materials (*Nature Materials* 2012) and high performance microporous membranes for separation of important environmental gases (*Nature Commun.* (2013, 2014)). In this presentation, we will discuss the science behind the materials used in developing such applications.

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1989-1993 MEng, Chemical Engineering, Imperial College.

Research Interests:

Material Transport in porous media, Cell Materials Interactions.

Selected Publications:

- Song, Q., Cao, S., Pritchard R., Terentjev, E., Al-Muhtaseb S.A., Cheetham A.K., Sivaniah E.*. Controlled thermal oxidative crosslinking of polymers of intrinsic microporosity for tunable molecular sieve membranes, *Nature Communications*. 5, Article number: 4813 (2014)
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Multi-scale Modeling for MEMS: from physical principles to engineering applications

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Micro- and nano-electro-mechanical systems (MEMS, NEMS) provide a challenging platform to realize micro-nanomechanics and microfluidics experiments at the smallest scales, with an unprecedented control on the experimental parameters. The impact of such technologies, for example in biology and medicine, is increasing at a fast pace. Our theory group at IEMN has developed several collaborations with the LIMMS-Cnrs Laboratory and the IIS, both in the University of Tokyo and world-leading experts in MEMS technologies. I will present here the results of our multiscale approach, combining atomic-scale molecular dynamics, mesoscale Monte Carlo simulations, macroscopic PDE and statistical mechanics models, for two relevant examples.

In a first case, the extreme plasticity observed in MEMS experiments on silicon nanowires [2] is explained in terms of a two-phase theoretical model,[2,3] describing the evolution of a nanocrystalline structure connected by a thin layer of amorphous material. Liquid-like flow in the amorphous is identified as the responsible for the exceptional elongation of the Si nanowires, in excess of 2000%. The continuum model is based on microscopic observations obtained from atomic-scale molecular dynamics simulations, of the tensile deformation of a model Si nanowire. Numerical solutions of stress-strain curves from the analytical model show a multi-stage deformation behavior, in excellent agreement with the experiments.

In a second example, we studied the response of both single DNA molecules and large DNA bundles, stretched by MEMS “nanotweezers”. The objective is to understand the failure of DNA fibers exposed to gamma-ray irradiation, to improve the specificity of cancer radiotherapy.[4] We developed combined Monte-Carlo simulations and statistical-mechanics modeling to describe the microscopic kinematics of the damage process. Analysis of the finite-size elasticity of a two-state model of single DNA molecules stretched at large applied forces,[5] demonstrate that the experimental force-extension curves can be described by a unique universal model, despite the differences in polymer size, structure, chemistry and rate-dependence of transition forces. Next, DNA bundle degradation induced by ionizing radiation is modeled by an assembly of parallel fibers, progressively damaged by a random population of breaks.[6] Fibers interact by means of a lateral viscoelastic coupling, thus retaining structural integrity even after substantial damage. Monte Carlo simulations of the Young's modulus degradation for increasing DNA damage density demonstrate a remarkable scaling shift between an exponential and a power-law regime. Analytical solutions of the model confirm this behavior, and provide a thorough understanding of the underlying physics.

[1] T. Ishida, F. Cleri et al., *Nanotechnology***22**, 355704 (2011)

[2] F. Cleri, T. Ishida, D. Collard, H. Fujita, *Appl. Phys. Lett.***97**, 153106 (2010)

[3] F. Cleri, *Int. J. Plasticity***37**, 31 (2012)

[4] G. Perret et al., *Engineering in Medicine and Biology Society*, 35th Conf. of IEEE, p. 6820 (2013)

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Education

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2004 Habilitation in Physics, University of Strasbourg, France

Professional Experience

2010 – present: Director of the Master School in Biophysics and Medical Physics, University of Lille I (France)

2006 – present: Full professor of Physics, University of Lille (France), and Group leader, IEMN Cnrs, Lille (France)

1992 – 2005: Senior scientist, Group leader, ENEA, Rome (Italy)

1985 – 1992: Staff Scientist, ENEA, Rome (Italy)

Visiting professor, ISS University of Tokyo (Japan) (09-12/2008)

Visiting professor, Rensselaer Polytechnic Troy, New York (USA) (01-04/2003)

Visiting scientist, University of Chicago, Argonne National Laboratory (USA) (06/1995 – 06/1998)

Visiting scientist, MIT Cambridge (USA) (06/1994 – 12/1994)

Associate Editor of “Applied Physics Letters”, and “European Physical Journal E (Soft Matter and Biological Physics)”

Fields of Research

Statistical mechanics of nanostructured and disordered materials; Biophysics and Nano-Bio interfaces; Multi-scale computer simulation of atomic and molecular systems

Publications

1. G. Copie, F. Cleri, Y. Makoudi, C. Krzeminski, M. Berthe, F. Cherioux, F. Palmino, B. Grandidier, *Surface-induced optimal packing of two-dimensional molecular networks*, Phys. Rev. Lett. **114** (2015) 066101
2. F. Manca, S. Giordano, P. L. Palla and F. Cleri, *Scaling shift in multicroaked fiber bundles*, Phys. Rev. Lett. **113** (2014) 255501
3. RS Prasher, XJ Hu, Y Chalopin, N Mingo, K Lofgreen, S Volz, F Cleri, *Turning carbon nanotubes from exceptional heat conductors into insulators*, Phys. Rev. Lett. **102** (2009) 105901
4. F. Cleri, S. R. Phillpot, D. Wolf and S. Yip, *Atomistic simulations of materials fracture and the link between atomic and continuum length scales*, J. Amer. Cer. Soc. **81** (1998) p. 501
5. F. Cleri and V. Rosato, *Tight-binding potentials for transition metals and alloys*, Phys. Rev. **B22** (1993), p. 22

Molecular separation by a free-standing and nanometer-thick membrane

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Biological lipid bilayer membrane is an ideal example for precise and efficient molecular separation. One of its characteristics is free-standing property with molecular thickness, and molecular scale phenomena become dominant in the direction of the membrane thickness. Thus, artificial membrane with a free standing properties and nanometer thickness would be a unique property different from conventional membrane. Based on this idea, we have developed functional free-standing nanomembranes with a centimeter-scale of lateral size (Fig.1).[1],[2] These membrane are manipulable macroscopically, event its thickness is a few tens nanometers.

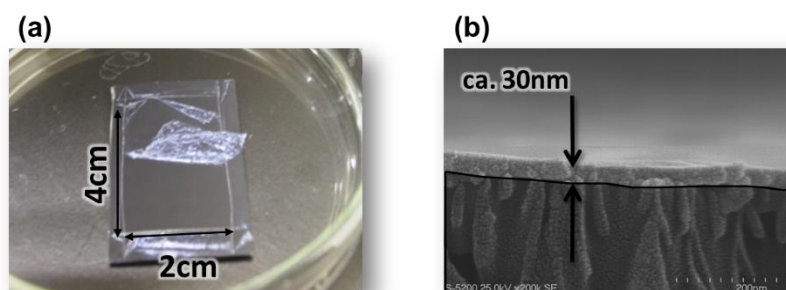


Figure 1. Free-standing nanomembrane (a) and the cross sectional image on a porous support (b)

We have succeeded to prepare a free-standing and ultrathin membrane with precise molecular filtration ability by designing nanochannels structures across a membrane. Our next target is to separate further small molecules, including CO₂ and gaseous molecules, because membrane separation of CO₂ is one of promising CO₂ capture technologies. In this scope, we have developed membranes composed of polymer and inorganic materials.

In polymeric nanomembranes, we have investigated cross linkable materials, such as an epoxy resin, urea and melamine derivatives, for the preparation of nanomembrane. In all case, we have succeeded to prepare free-standing membrane with a few tens nanometer thick, and the gas permeance of each membrane was investigated.

In inorganic membrane, we employed the composite materials composed of titanium alkoxide carboxylic derivatives, such as phthalic acid, to control the gas selectivity of the membrane. Based on a spin-coating process, titania composite membrane with the thickness of 100 nm or less was prepared on a PDMS support. Some composite membrane, show preferential CO₂ permeation over nitrogen.

In membrane separation, the thickness plays an important role for the efficient separation. Further thinning to reach the thickness of a biological lipid membrane is our challenge to create ideal membrane separation based on molecular dynamics.

[1] S. Fujikawa, E. Muto, and T. Kunitake, *Langmuir*, 25(19), 11563-11568 (2009)

[2] S. Fujikawa, E. Muto, and T. Kunitake, *Langmuir*, 23(8), 4629-4633 (2007)

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Education

- Bachelor: Faculty of Engineering, Kyushu University (1994)
- Master: Graduate School of Engineering, Kyushu University (1996)
- Ph.D.: Graduate School of Engineering, Kyushu University (1999)

Professional Experience

- Research Fellow of the Japan Society for the Promotion of Science, Department of Chemistry, Yale University (Connecticut, USA), 1999 - 2000
- Special Postdoctoral Researcher, RIKEN (Saitama, Japan), 2000-2004
- Deputy of Laboratory Head, RIKEN (Saitama, Japan), 2004-2011
- Partner and Board Member, NanoMembrane Technologies Inc. (Saitama, Japan), 2007-present
- Adjunct Associate Professor, Department electronic Chemistry, Tokyo Institute Technology (Kanagawa, Japan), 2008-2012
- Associate Professor, Kyushu University, 2011-Present

Fields of Research

Surface nanostructure, nanometer-thick membrane, nanofabrication

Publications

1. Yamada Y., Yuyama Y., Sato T., Fujikawa S., Uozumi Y., *Angew. Chem. Int. Ed.*, **53**, 1, 127-131(2014)
2. Taniguchi I, IohD.,Fujikawa S., Watanabe T., Matsukuma Y., Minemoto M., *Chem. Lett.*, **43**(10), 1601-1603(2014)
3. Akamatsu N., Tashiro W., Saito K., Mamiya J., Shishido A., Kinoshita., Ikeda T., Takeya J., Fujikawa S., Priimagi A., *Scientific reports*, **4**, 5377 (2014)
4. Kubo W., Fujikawa S., *Nano Letters*, **11**(1), 8-15(2011).
5. Fujikawa S., Muto E., Kunitake T., *Langmuir*, **25**(19), 11563-11568 (2009)

Atomic Scale Simulations in Materials Science and Biochemistry

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The common denominator of this presentation is a general overview is the development, implementation and application of the most advanced computational tools in the field of first principles and hybrid QM/MM (quantum mechanics / molecular mechanics) dynamical simulations techniques. These represent nowadays a general tool to perform accurate virtual experiments able to complement and to extend the insight provided by actual experiments. Free energy sampling techniques can be efficiently coupled to these methods to simulate activated processes and to workout reaction pathways. The range of applications where these methodologies are exploited extends from solid state physics to surface chemistry and to biochemical reactions. We shall focus on selected examples, corresponding to projects done in collaboration with major Japanese universities and laboratories. More specifically, patterning of graphene-based materials [1] and enzymatic reactions for green chemistry [2,3] will be presented as representative examples of atomic-scale driven processes having a macroscopic impact in nanotechnology and life science.

[1] Koizumi K., Boero M., Shigeta Y., Oshiyama A., *J. Phys. Chem. Lett.* **4**, 1592 (2013)

[2] Kamiya K., Baba T., Boero M., Matsui T., Negoro S., Shigeta Y., *J. Phys. Chem. Lett.* **5**, 1210 (2014)

[3] Baba T., Boero M., Kamiya K., Ando H., Negoro S., Nakano M., Shigeta Y., *Phys. Chem. Chem. Phys.* **17**, 4492 (2015)

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Education

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Professional Experience

1/1995~7/1995 - Post-Doc at EPFL-IRRMA (Switzerland)
8/1995~4/1996 - Post-Doc at IBM Zurich Research Laboratory (Switzerland)
5/1995~5/1998 - Post-Doc at Max-Planck-Institut, Stuttgart (Germany)
5/1998~3/2001 - Post-Doc. JRCAT-AIST, Tsukuba (Japan)
4/2001~8/2002 - NEDO Fellow at AIST-RICS, Tsukuba (Japan)
9/2002~12/2008 - Associate Professor at University of Tsukuba (Japan)
1/2009 ~ to date – Research Director at IPCMS UMR 7504 CNRS - University of Strasbourg, Strasbourg (France)

Fields of Research

Molecular simulations and modeling in condensed matter and biosciences. Visiting Full Professor at University of Tokyo – Computational Materials Science Initiative (CMSI) Project member (Japan); Visiting Full Professor at European Center for Atomic and Molecular Calculation - CECAM (Switzerland). Scientific director of the HPC Meso-Center (Equipex EQUIP@MESO). Author of more than 130 publications, among which 112 original research papers, 7 review articles, 6 book chapters, and 22 proceedings of international conferences. Results of ISI-Web-of-Science of 27/03/2015: Number of citations: 3343, h-index: 31

Publications

(Selection of 5 relevant publications)

1. F. L. Gervasio, M. Boero and M. Parrinello, *Angew. Chem. Int. Ed.* **45**, 5606 (2006)
2. M. Boero, T. Ikeda, E. Ito and K. Terakura, *J. Am. Chem. Soc.* **128**, 16798 (2006)
3. B. W. Heinrich, L. Limot, C. Iacovita, M. V. Rastei, J.-P. Bucher, D. Mbongo Djimbi, C. Massobrio and M. Boero, *Phys. Rev. Lett.* **107**, 216801 (2011)
4. K. Koizumi, M. Boero, Y. Shigeta and A. Oshiyama, *J. Phys. Chem. Lett.* **4**, 1592 (2013)
5. K. Kamiya, T. Baba, M. Boero, T. Matsui, S. Negoro, Y. Shigeta, *J. Phys. Chem. Lett.* **5**, 1210 (2014)

Mathematics-Materials science Cooperation

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The major research direction at AIMR is to develop cooperation between mathematics and materials sciences to achieve revolutionary new concept of materials and their functionalization. In this talk, some examples of the collaboration between mathematics/theory and materials sciences are introduced.

The first example is the topics of atomic structure analysis of metallic glasses with collaboration of angstrom beam electron diffraction and computational homology. The new approach provides a general method for a clear description of short to mid range orders of amorphous materials beyond conventional two-body distribution functions. Next topics is on the recent results of nano-level structuring of water/aqueous solution obtained by the first-principles MD calculations as well as AFM observation. It will be shown that regular hydrogen bond(HB) chains or their rings play an important role of non-local molecular splitting of water causing significant influences on (electro-)chemical processes of water/aqueous solution. Final topics is on the competing wave-like or particle-like features of electron/hole transport in middle size molecules or long chain molecules bridging between electrodes. As wave-nature predominating cases, we will introduce theoretical prediction of large internal loop currents in fullerene, triangular graphene, certain kinds of CNT tori, and on a particle-nature predominating case, we show the Frank-Condon blockade of C_{60} between nano-electrodes. Finally for the case of long helical polyacetylene, Poly(octyloxyphenylacetylene) POOPA, we can see a transition from the wave-like to particle like diffusion by analyses with time dependent wave-packet diffusion method. A unique feature, multi pass transport, characteristic of helical structures is found.

[1].Mitsutake M, Yano K, Tsukada M; in press, *J. Phys. Chem.2015* , DOI:10.1021

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Education

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1965 BSc, solid state physics (Theory) University of Tokyo

Professional Experience

Specially appointed Professor	
Administrative Director, at AIMR, Tohoku University,	2012-2015
Professor, PI, at AIMR, Tohoku University	2008-2012
Professor at Graduate School of Advanced Science and Technology, Waseda University	2004-2008
Professor at Faculty of Science, University of Tokyo	1991-2004
Associate Professor at Faculty of Sci., Univ. of Tokyo	1982-1991
Associate professor at Institute for Molecular Science	1976-1982
Research Associate at Faculty of Sci., Univ. Tokyo	1970-1982

Fields of Research

Theory of SPM and nano-structures, modeling and computations

Publications

1. Hamada I, Shimizu R, Ohsawa T, Iwaya K, Hashizume T, Tsukada M, Akagi K, Hitosugi T, Journal of the American Chemical Society, **136** 17201 (2014)
2. H.Tamura, Tsukada M, Ishii H, Kobayashi N, and Hirose K, Physical. Review. **B87**, 155305 (2013)
3. Tamura H, Tsukada M, McKenna, K.P, Shluger A.L, Ohkubo T, Hono K, Physical Review **B 86**, 195430 (2012)
4. Tsukada M, Masago A, Shimizu M, Journal of Physics, Condensed Matter, **24** 984002 (2012)
5. Araidai M, and Tsukada M, Physical. Review. B84, (2011) 195461

WITH: Wireless communication using TeraHertz plasmonic-nano ICT devices

The Japanese-French initiative on plasmonic nano-device technologies for ultra-broadband wireless communications using “terahertz” waves

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The strongly increasing demand for higher-data-rate wireless communication owing to the trend of a ubiquitous ICT society has led us to explore new frequency resources higher than any existing wireless communication band, approaching “terahertz (THz)” or 1000 GHz. For example in the very near future super-HDTV will become available for which over 40-Gbit/s wireless transmission over carrier frequencies of 400GHz and higher will be needed. THz and sub-THz waves can be considered for a wide aspect of last-mile, short-distance free-space high data-rate communication purposes using a several existing atmospheric windows with low attenuation (0.1dB/10m). However the feasibility of very high data-rate transmission with sub-THz to THz carrier is still an open question. There are two main problems: i) how to generate and modulate the sub THz signals, and ii) how to detect them. **Showing the feasibility and demonstrating the first high data rate ~40-Gbit/s communication prototypes at unexplored frequency range from 400 to 900 GHz by testing and improving existing devices and developing novel plasmonic nano-devices is the main goal of this ‘WITH’ project.**

In order to break through the speed limit of conventional carrier transit-type electron devices, we considered THz plasma oscillations in the 2D (two-dimensional) in nanostructures as a new physical mechanism of operation to realize i) frequency-tunable, room-temperature operating coherent monochromatic THz sources, ii) fast, detection of coded THz carrier waves, and iii) 10-40-Gbit/s intensity modulators for sub-THz and THz carrier signals. The fundamental structure of those devices was based on the nanometer high electron mobility transistors (HEMT's) and applicant's original dual-grating-gate (DGG) HEMT structures. Novel advanced device structures integrated with antennas were developed and integrated into the real devices/demonstrators. We developed also new/improved models of the most competitive existing THz sources based on the use of UTC-PD's (Uni-Travelling Carrier PhotoDiodes) as an alternative existing reference standard of state-of-the-art technology. Real test-bed sub-THz and THz wireless transmitter/receiver frontend devices were designed and integrated to demonstrate up to 40-Gbit/s class wireless communication, verifying the feasibility of the ultra-broadband THz wireless communications under a complementary, co-lateral collaboration between Japanese and French teams.

The major achievements on this JST-ANR WITH project are (i) the development of ultrahigh-sensitive broadband plasma-wave detectors featured by a newly-invented asymmetric dual-grating gate (A-DGG) structure, and (ii) Building up 200-720-GHz class wireless communication test systems demonstrating world-record 40-Gbit/s error-free transmission of HDTV signals using THz frequencies.

The project accompanied/reinforced international research network (GDRI) with many other partners from Poland, France, Japan and Russia, leading to creation of EU founded COST action MP1204 **TERA-MIR Radiation: Generation, Detection and Applications.**

[1] Sci. Technol. 3, 63 (2013); W. Knap et al Nanotechnology 24, 214002(2013), S. Blin et al., IEEE Electron Device Lett. 33, 1354 (2012) ; J. Oden et al., Opt. Exp. 21, 4817 (2013) ; T. Nagatsuma et al., Opt. Exp. 21, 23736 (2013).

Illustration

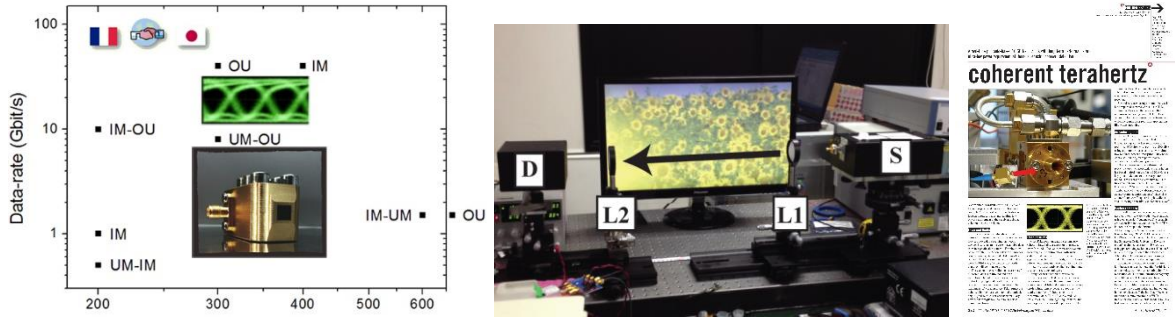


Fig. 1. Left: benchmarking the WITH project achievements for data rate vs. carrier frequency. Center : photograph of the uncompressed HD video transmission showing the frequency-multiplied source on the right, the plasma-wave receiver on the left (inside its electromagnetic shielding box), and two Teflon lenses in between for collimating and focusing. The source amplitude is modulated by a real-time high-definition and uncompressed video signal. Transmitted signal is observed on the TV screen at the background. Right: latest publication in IEE Electronics Letters has been highlighted as a “Featured Issue” of an excellent France-Japan collaborative work.

Factual information

The WITH project was an experimental research project exploring the limits of wireless communication using innovative technologies. It was coordinated by W. Knap (CNRS – Montpellier) in France and by T. Otsuji (Tohoku University) in Japan. It was associated with 3 French laboratories from CNRS-Univ. Montpellier (Montpellier), IEMN (Lille) and Univ. Savoie (Chambéry), as well as 3 Japanese laboratories from Tohoku University (Sendai), Osaka University (Osaka), and RIKEN (Sendai). The project started on November 2010 and lasted 36 months. ANR grant amounted to 969,996 € (135.8 M¥) and JST grant amounted to 141 M¥ (1,007,142 €) for a total budget of 1,977,138€ (276.8 M¥) at an exchange rate of 1 € = 140 ¥.

Development and characterization of nano-composite capacitors based on tantalum-polymer

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The development of conducting polymers, especially in terms of environmental stability, imposes organic compounds as a new technology for electronic devices in specific areas of activity such as space, aerospace or defence. Following this trend, currently tantalum capacitors based on manganese dioxide cathode have been recently improved by the replacement of this cathode with a conducting polymer. Polymer Tantalum capacitors consist of a Ta anode sintered from Ta powder, an anodic oxide film of Ta as a dielectric, and a conductive polymer cathode typically made of poly 3,4-ethylenedioxythiophene (PEDOT). Until recently, capacitors based on PEDOT cathode have been optimized only for low capacities by in-situ polymerization. The next step is to reach higher capacities and improve the performance of capacitors using the conductive polymer. Our work is focus on the efficient insertion of the polymer into the device. The main study is the characterization of tantalum polymer capacitor via physico-chemical investigations carried out from the tantalum powder to conducting polymer and complete capacitor. We first studied the microstructure of tantalum network of existing capacitors by mercury porosimetry and observations by both scanning and transmission electronic microscopy. Afterwards, the solution containing PEDOT has been investigated by different techniques to determine parameters for the imbibition of tantalum anodes. This laboratory characterization is complemented by an assessment of the electrical performance of samples within the company. All this work has contributed to a new range of tantalum polymer capacitors available since the beginning of 2014 in the product catalogue of Firadec Company.

Synthesis of Ni-poor NiO nanoparticles for DSSC-p applications

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Over the last decade, p-type semiconductors (SC) have known a renewed interest. Indeed these materials may have potential applications for light-emitting diodes, transistors, solar cells, etc. Since the achievement of the first Dye Sensitized Solar Cells by Grätzel ^[1] in 1991 a new generation of solar cells has been developed ^[2] where the n-type SC is replaced by a p-type one. This leads to the photo-injection of holes instead of electrons in the circuit. To date nickel oxide (NiO) is the reference p-type semiconductor. However yields are still far from those of DSSC-n and many studies aim to replace NiO by other systems such as CuAlO₂, CuGaO₂, CuCrO₂ or NiCo₂O₄ nanoparticles. Following our recent synthesis of N doped ZnO with stabilization of p-type charge carriers ^[3], we focus now on the preparation of N doped NiO nanoparticles to improve the p-type conductivity of NiO. We study here the chemical reactivity of a nickel oxyhydroxide precursor under air and ammonia that conducts to nanostructured Ni-poor NiO.

[1] B. O'Regan, M. Grätzel, *Nature* **353**, 737-740 (1991).

[2] F. Odobel, L. Le Pleux, Y. Pellegrin, E. Blart, *Acc. Chem. Res.*, **43**, 1063–1071, (2010).

[3] B. Chavillon, L. Cario, A. Renaud, F. Tessier, F. Cheviré, M. Boujtita, Y. Pellegrin, E. Blart, A. Smeigh, L. Hammarström, F. Odobel, S. Jobic, *J. Am. Chem. Soc.* **134**, 464-470 (2012).

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**Education**

2013-2016 PhD, Chemistry, Université de Rennes 1

2012 Master degree in Solid State Chemistry and Materials, Université de Rennes 1

Fields of Research

Oxide/Nitride

P-type semiconductors

Nanoparticles

DSSC

Dynamics of Soft Crystals and Defects

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The dynamic pattern formation is ubiquitous in nature. The patterns often appear as spatially ordered states, which consist of patches of various shapes. These are associated with local symmetry left after breaking rotational symmetry. In this presentation, we try to show our recent effort to understand defect dynamics of crystals described as dynamics of patterns created by phenomenological nonlinear partial differential equations (PDE). We call it as *soft* crystals.

Such *soft* crystals may have rotational defects (disclination) as well as translational defects (dislocation), which are of relevance for macroscopic properties of materials. The classification of these defects has a long history and it is relatively well understood what kind of defects appears depending on the local symmetry. Compared with the static structure, dynamics of defects is less well understood. In order to tackle this problem, we use the phase-field-crystal-type PDEs and analyze their motion and deformation under nonequilibrium states.

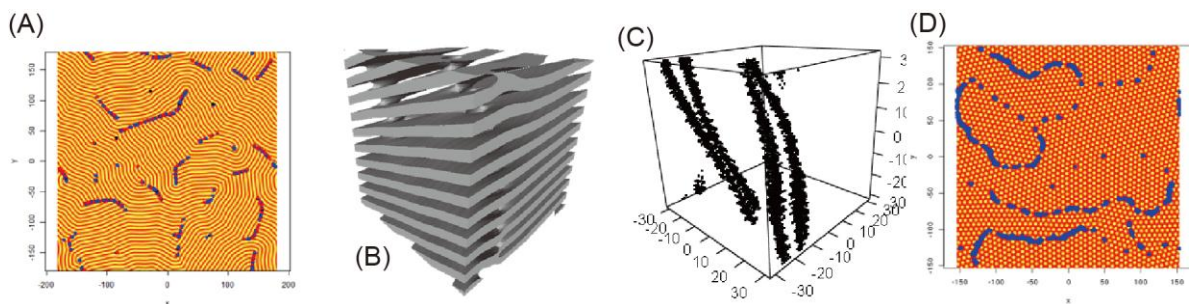


Fig. 1. (A) Lamellar and (D) hexagonal patterns in two dimensions. Topological defects (dislocations and disclinations) are also shown. (B) A lamellar pattern in three dimensions with screw dislocation line extracted (C).

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Education

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Professional Experience

Research Fellow of the Japan Society for Promotion of Science for Young Scientists (DC1), Department of Physics, Kyoto University, Japan, 2004-2007

Visiting Fellow, Département de recherche fondamentale sur la matière condensée (DRFMC), CEA-Grenoble, France, 2005-2006

Research Fellow of the Japan Society for Promotion of Science for Young Scientists (PD), Department of Physics, the University of Tokyo, Japan, 2007-2010

Visiting Fellow, PhysicoChimie Curie UMR 168, Institut Curie, Section recherche, France, 2007-2008

Research Fellow, Fukui Institute for Fundamental Chemistry, Kyoto University, Japan, 2010-2011

Assistant Professor, WPI-AIMR, Tohoku University, Japan. 2011-present

Fields of Research

Active Soft Matter, Nonlinear Dynamics, Theoretical Biology

Publications

1. Yoshinaga N., *Physical Review E* **89** 012913(2014)
2. Yoshinaga N., Nagai K. H., Sumino Y., and Kitahata H., *Physical Review E* **86** 016108(2012)
3. Yoshinaga N., Joanny J.-F., Prost J., and Marcq P., *Physical Review Letters* **105** 238103(2010)
4. Jiang H.-R., Yoshinaga N., and Sano M., *Physical Review Letters* **105** 268302(2010)
5. Yoshinaga N., Kats E. I., and Halperin A., *Macromolecules* **41** 7744-7751(2008)

Equivalence Class Sampling for Molecular Self-Assembly on Surfaces

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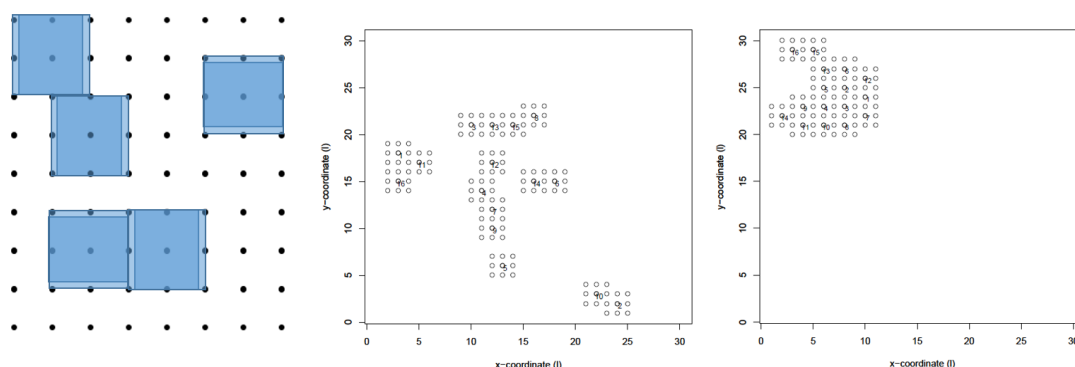
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An important problem for materials science is to predict *a priori* what kinds of structures are formed by self-assembly of molecules on metal surfaces. This presentation will introduce a mathematical model for exploring the thermodynamic stability of molecular assemblies on periodic surfaces. This model considers N square blocks on a finite square lattice, each with one of two orientations. The blocks have dimension $2l \times 2l$, where l is the lattice constant, and the interaction energy between the blocks depends upon their relative alignment and orientation (left-hand figure). This 'block assembly model' captures some key aspects of bottom-up fabrication of graphene nanoribbons from organic precursors on copper and gold surfaces (Han *et al.* *ACS Nano***8**, 2014, 9171).

The block assembly model allows for a rich variety of block assembly structures, and predicting which ones dominate at equilibrium ('optimising' the model) is a difficult problem. In particular, naïve application of typical Monte Carlo methods fail spectacularly, as the blocks quickly gather into a large number of small, mildly stable assemblies and do not adopt other configurations on the simulation time-scale (middle figure). We are developing a new technique called 'equivalence class sampling' for optimising the block assembly model at equilibrium. Equivalence class sampling makes use of the fact that a very large number of the block configurations can be made equivalent by simply rotating the block assemblies and translating them about the lattice. Instead of considering every possible block configuration, we can therefore consider the relatively small number of configuration 'classes', without losing any information on the problem. This affords a major improvement in the efficiency of optimising the block assembly model, however there is a price: equivalence class sampling algorithms turn out to be difficult to set-up. We are developing an algorithm called 'reduction-extension', and early calculations show rapid convergence to very large, thermodynamically stable island structures (right-hand figure).



Left: Sketch of the block assembly model. The two edge designs on the blocks indicate that the sides of the blocks possess different chemical characteristics.

Middle: State of a typical Monte Carlo sampling algorithm after 10^6 steps.

Right: State of the Equivalence Class sampling algorithm after 7000 steps.

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Fields of Research

Stochastic modeling and Monte Carlo simulation for problems in chemical physics.

Publications

1. Packwood D. M., Oniwa K., Jin T., Asao N., Charge transport in organic crystals: Critical role of correlated fluctuations unveiled by analysis of Feynman diagrams. *Journal of Chemical Physics*, **142**, 144503 (2015)
2. Packwood, D. M., Jin, T., Fujita, T., Chen, M. W., Asao, N., Mixing time of molecules inside of nanoporous gold. *SIAM Journal on Applied Mathematics*, **74**, 1298 (2014)
3. Packwood D. M., Shiraki, S., Hitosugi, T., Effects of Atomic Collisions on the Stoichiometry of Thin Films Prepared by Pulsed Laser Deposition. *Physical Review Letters* **111**, 036101 (2013)
4. Packwood D. M., Reaves, K. T., Federici, F. L., Katzgraber, H. G., Teizer, W., Two-dimensional molecular magnets with weak topological invariant magnetic moments: mathematical prediction of targets for chemical synthesis. *Proceedings of the Royal Society A* **469**, 20130373, (2013)
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Fabrication and characterization of nanoscale heterogeneous interfaces of epitaxially grown anatase-type TiO₂ on CeO₂ nanocubes

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Heterogeneous interfaces have been drawing much attention so far. Particularly, nanoscale heterogeneous interfaces are attractive because of quantum confinement effects. To fabricate nanoscale heterogeneous interfaces, we use nanocrystals that fixed to the surface as a nanoscale substrate. In order to apply nanocrystals to the surface, at least three things have to be considered. 1) Dispersing nanocrystals in a solvent. 2) Self-assembling the nanocrystals on the substrate with drying the solvent. 3) Fixing the nanocrystals on the substrate. Among these processes, necessary interaction between the inorganic cores, modifiers, solvent, and the substrates is totally different. This could then lead to a difficulty to apply nanocrystals to the surface macroscopically uniformly.

We have so far synthesized decanoic acid modified CeO₂ nanocubes to disperse those nanocubes in cyclohexane [1] and modified silicon substrates so that chemical bonding could be constructed between the nanocubes and those modified surfaces to fix them during self-assembly. [2, 3] Once the nanocubes are fixed to the substrate, monolayer structure of nanocubes can be fabricated macroscopically by washing residual nanocubes on the monolayer.

In this presentation, nanoscale epitaxy for fabricating nanoscale heterogeneous interfaces is demonstrated combining bottom-up and top-down processes. TiO₂ sputtered was selectively nucleated and grown on individual CeO₂ nanocubes used as a nanoscale substrate fabricating TiO₂/CeO₂ tandem nanocrystals (Fig. 1). The heterogeneous interfaces were then fabricated between anatase TiO₂ (001) and CeO₂ (001) nanocube such that the anatase TiO₂ [110] directions were parallel to the CeO₂ [100] directions. [4] The result of ultraviolet-visible spectroscopy of TiO₂/CeO₂ tandem nanocrystals will be also discussed in this presentation.

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- [2] Hojo et. al *Chem. Mater.* 22, 1862 (2010).
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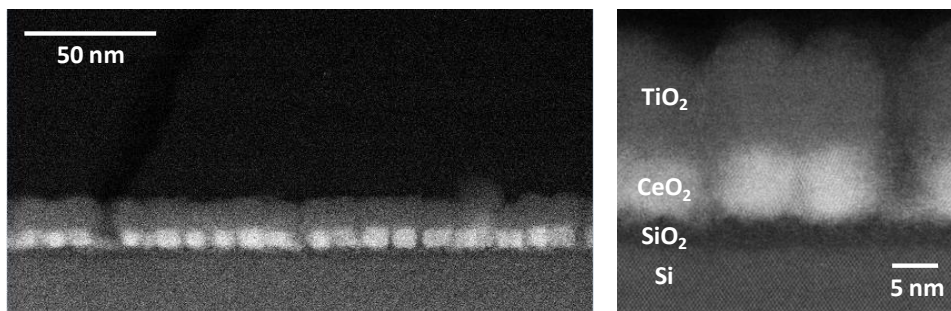


Figure 1. Cross-sectional transmission electron microscope images of heterogeneous interfaces between anatase TiO₂ and CeO₂ nanocubes.

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Assistant Professor, Advance Institute for Materials Research, Tohoku University, 2008-present

Fields of Research

Nanomaterials, Thin film deposition

Publications

1. Hwang E. T., Sheikh K., Orchard K. L., **Hojo D.**, Radu V., Lee C.-Y., Ainsworth E., Lockwood C., Gross M. A., Adschiri T. Reisner E., Butt J. N., Jeuken L. C., *Adv. Funct. Mater.***25**, 2308 (2015).
2. **Hojo D.**, Togashi T., Ohsawa T., Saito M., Wang, Z., Sakuda Y., Asahina S., Ikuhara Y., Hitosugi T., Adschiri T., *Cryst. Growth Des.***14**, 4714 (2014).
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4. Dejhosseini M., Aida T., Watanabe M., Takami S., **Hojo D.**, Aoki N., Arita T., Kishita A., Adschiri T., *Energy & Fuels***27**, 4624 (2013)
5. **Hojo D.**, Togashi T., Iwasa D., Arita T., Minami K., Takami S., Adschiri T., *Chem. Mater.***22**, 1862 (2010).

Nanoscale orientation control of organic semiconductor thin films on amorphous substrates by graphoepitaxy

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Graphoepitaxy, in-plane oriented crystal growth on artificial microstructures, was discovered about 40 years ago in inorganic materials [1]. We applied this technique to organic semiconductors in order to obtain in-plane oriented films and improve the performance of organic thin film transistors (OTFTs).

By means of electron beam lithography and dry-etching, periodic grooves were fabricated on thermally oxidized silicon substrates; the pitch and depth of the grooves were 400 nm and 10 nm, respectively. The grooved substrate after UV/ozone cleaning (hydrophilic surface condition), or further treated with hexa-methyl-disiloxane (HMDS) (hydrophobic surface condition), was loaded into an ultrahigh vacuum chamber, and an α -sexithiophene (α -6T; $C_{24}H_{14}S_6$) thin film was grown on the substrate by molecular beam deposition. Atomic force microscopy (AFM) images of the substrate and grown thin films are shown in Fig. 1.

On the microgrooved surface, one-dimensional chain-like patterns of α -6T grains were observed along the grooves by AFM. Morphological analysis of crystal grains and grazing-incidence x-ray diffraction (GIXD) revealed that in-plane oriented growth (graphoepitaxy), b -axis \parallel grooves (c -axis \perp grooves) on hydrophilic surface and b -axis \perp grooves (c -axis \parallel grooves) on hydrophobic surface, was achieved [2,3]. The orientational change is caused by the interaction between α -6T and molecules terminating the groove walls, and can be used for nanoscale orientation control. Some tests confirming the effect of graphoepitaxy on the performance of OTFTs have been carried out [4]. Furthermore, we investigated the possibility of graphoepitaxy using edges of metal electrodes [5].

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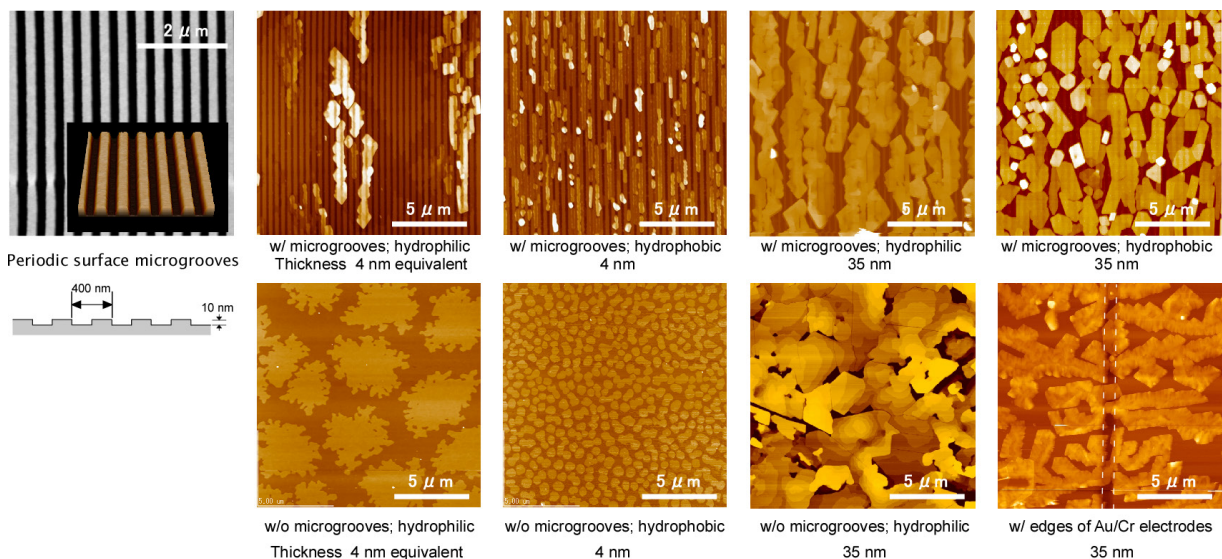


Fig. 1 AFM topographies showing morphological variation of α -6T thin films grown on substrates with/without microgrooves, with different film thickness and surface condition.

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Fields of Research

- ◆ Oriented film growth of organic semiconductors by graphoepitaxy
- ◆ Organic field effect transistors and their ambipolar characteristics
- ◆ Light emission properties of organic semiconductors and devices
(Others: Mineralogy, Petrology, Experimental petrology, Cement chemistry, Surface science)

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9. K. Oniwa, T. Kanagasekaran, T. Jin, Md. Akhtaruzzaman, Y. Yamamoto, H. Tamura, I. Hamada, H. Shimotani, N. Asao, S. Ikeda and K. Tanigaki, *J. Mater. Chem. C* **1**, 4163-4170 (2013).

Novel Nanocomposites Based on Silica via Reverse Microemulsions and Lanthanide-Based Coordination Polymers

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Among the arising nanotechnologies in catalysis, optical or biological, multifunctional nanoparticles with complex architecture constitute one of the most promising and studied research fields. In our work, the control of the luminescence property of nanomaterials is mandatory for applications in photonic and biomedical areas. By exploiting important colloidal phenomena, the goal of our work is to synthesize new luminescent and stable nanomaterials.

This contribution highlights our efforts to elaborate and to characterize various colloidal nanostructures based on different luminophors such as: lanthanide coordination polymers or $\gamma\text{-Fe}_2\text{O}_3\text{-Mo}_6\text{X}_{14}\text{@SiO}_2$ or $\gamma\text{-Fe}_2\text{O}_3\text{-Mo}_6\text{X}_{14}\text{@SiO}_2\text{@Au}$.

In the first part, we will summarize our results on the synthesis and characterization of luminescent $\text{Mo}_6\text{X}_{14}\text{@SiO}_2$ colloidal solution. Such nanoparticles including Mo_6X_{14} metal atom clusters (MC) as phosphors are good candidate for photonic crystal or bioimaging knowing that the red/infrared Mo_6 emission range could be selectively transmitted through tissues due to the low absorption at these wavelengths. Moreover, they generate singlet oxygen under irradiation, what is of particular interest for photodynamic therapy. In addition, we will show the possibility to encapsulate $\gamma\text{-Fe}_2\text{O}_3$ and luminescent molybdenum clusters units in silica nanoparticles through a W/O microemulsion process and the evolution of the luminescence properties as a function of the size of the magnetic core.

To our $\gamma\text{-Fe}_2\text{O}_3\text{-Mo}_6\text{X}_{14}\text{@SiO}_2$ MPs, small gold nanoparticles can be deposited on the surface of silica NPs allowing the preparation of gold nanoshells. Thus, thanks to the strong absorption of the plasmon band in the visible region, gold NPs can convert the absorbed light into heat, allowing the local destruction of cancer cells.

In the second part, we will show the possibility to stabilize solutions of polymer coordination nanoparticles by solvation in a green chemistry solvent. For more than a decade, lanthanide-based coordination polymers have attracted great attention, because of their topologies coupled with their great potential applications in luminescence and molecular magnetism. These solutions exhibit intense luminescence using very little quantities of heteronuclear lanthanide terephthalate coordination polymers and are stable over time: no particle aggregation or decrease in luminance is observed.

The real challenge was to synthesize a non-toxic solution that combines the luminescence of the clusters in the NIR and lanthanide-based coordination polymers so it would be useful in several fields such as: nanomedicine, magnetic resonance imaging, fluorescence microscopy and to create luminescent surfaces.

Preparation of Nitrogen doped ZnO thin films by colloidal route

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Zinc oxide is a material of great interest exhibiting pigmental, photocatalytic, piezoelectric, antibacterial, or varistor properties that have already been developed in many different fields of industry. Still novel applications emerge in various domains but they often require the preliminary stabilization of a p-type ZnO counterpart to the natural n-type ZnO to be stimulated. In optoelectronics for instance, the high optical transparency of ZnO thin films coupled with their high electrical conductivity and their strong room temperature luminescence could indeed open up the door to revolutionary technologies as transparent electrodes in solar cells and flat panel displays, light emitting diodes, lasers, etc. We have previously reported the stabilization of p-type nitrogen doped ZnO nanoparticles (ZnO:N) obtained through the decomposition of zinc peroxide (ZnO₂) at low temperature under ammonia flow [1]. Our objective is now to extend these results to the realization of p-type ZnO thin films by colloidal route in order to achieve n-ZnO/p-ZnO:N homojunctions which would lead to various applications in optoelectronics. The aim of the present work is to prepare nitrogen doped ZnO thin film by thermal decomposition of ZnO₂ films obtained by chemical conversion of ZnO colloidal thin films.

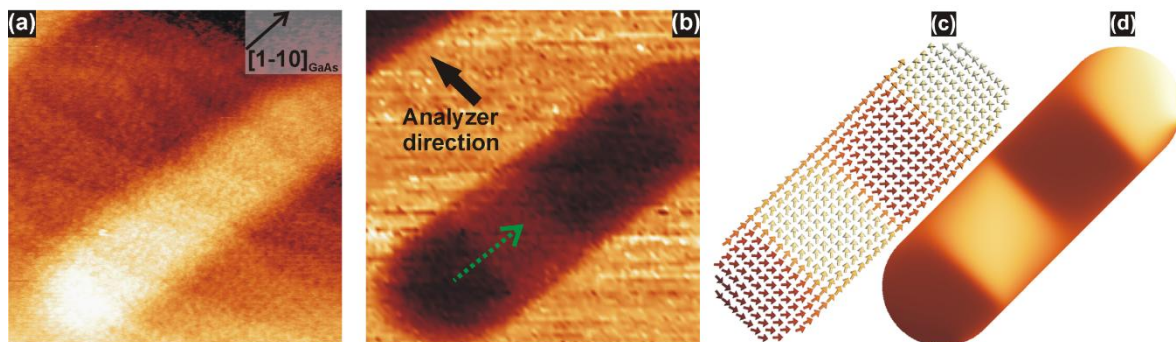
[1] B. Chavillon, L. Cario, A. Renaud, F. Tessier, F. Cheviré, M. Boujtita, Y. Pellegrin, E. Blart, A. Smeigh, L. Hammarström, F. Odobel, S. Jobic, *J. Amer. Chem. Soc.* **134**, 464-470 (2012)

Quantitative Ballistic Electron Magnetic Microscopy: magnetic imaging of buried nanostructures with a sub-nanometric lateral resolution

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We demonstrate quantitative ballistic electron magnetic microscopy (BEMM) imaging of simple model Fe(001) nanostructures. We use in situ nanostencil shadow mask resistless patterning combined with molecular beam epitaxy deposition to prepare under ultra-high vacuum conditions nanostructured epitaxial Fe/Au/Fe/GaAs(001) spin-valves. In this epitaxial system, the magnetization of the bottom Fe/GaAs(001) electrode is parallel to the [110] direction, defining accurately the analysis direction for the BEMM experiments. The large hot-electron magnetoresistance of the Fe/Au/Fe/GaAs(001) epitaxial spin-valve [1] allows us to image various stable magnetic configurations on the as-grown Fe(001) microstructures with a high sensitivity, even for small misalignments of both magnetic electrodes. The angular dependence of the hot-electron magnetocurrent is used to convert magnetization maps calculated by micromagnetic simulations into simulated BEMM images. The calculated BEMM images and magnetization rotation profiles show quantitative agreement with experiments and allow us to investigate the magnetic phase diagram of these model Fe(001) microstructures [2]. Finally, magnetic domain reversals are observed under high current density pulses. This opens the way for further BEMM investigations of current-induced magnetization dynamics.



1400*1400nm² STM image (a) and corresponding BEMM image (b) of a nanostructured stadium-shaped Fe/Au/Fe/GaAs(001) spin-valve. Note the presence of 4 magnetic domains in the Fe nanostructure. OOMF micromagnetic simulation of the 4 domains state (c) which was used to simulate (d) the experimental BEMM image.

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Nano-segregation and dynamics of ter-butanol/toluene binary liquids confined in mesoporous materials

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Different mesoscopic structures have been observed in binary mixtures of alcohol, often related to their incomplete mixing at the molecular level in apolar solvent or in aqueous solution. Recent neutron diffraction studies have revealed that the fully miscible ter-butanol/toluene binary mixtures form supra-molecular assemblies under confinement in the straight and mono-disperse rigid channels of mesoporous MCM-41 and SBA-15 silica molecular sieves. Indeed, systematic H/D contrast matching experiments suggest the possible formation of a surface-induced nano-segregation of the two components (core-shell structure) (Fig.1). Quasielastic neutron scattering experiments (BS and TOF) have been performed to assess the molecular dynamics of these nano-segregated mixtures, aiming to disentangle the main structural relaxation related to the ‘macroscopic’ glass transition from putative distinct modes arising from the different nano-segregated regions. Indeed, BS fixed window scans performed on IN16 and IN10 reveals the composition dependence of the glass transition of the confined mixture around 150 K, while at high temperature the slow dynamics of the TBA component is probed (Fig.2).

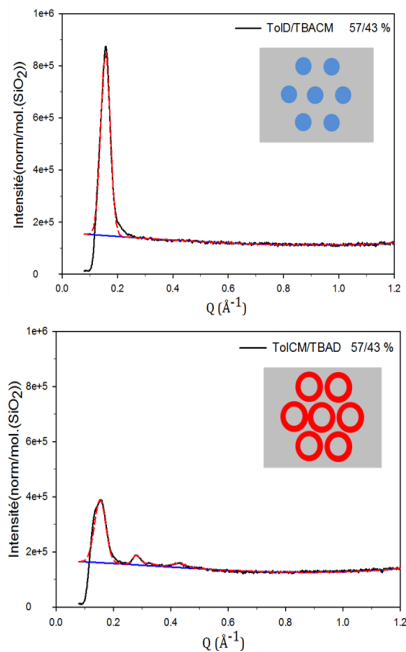


Fig.1. Neutron diffraction of TBA/TOL mixtures confined in MCM-41 with the same chemical but different isotopic compositions. The modulation of the MCM-41 Bragg peaks intensity reflects the radial nanostructure.

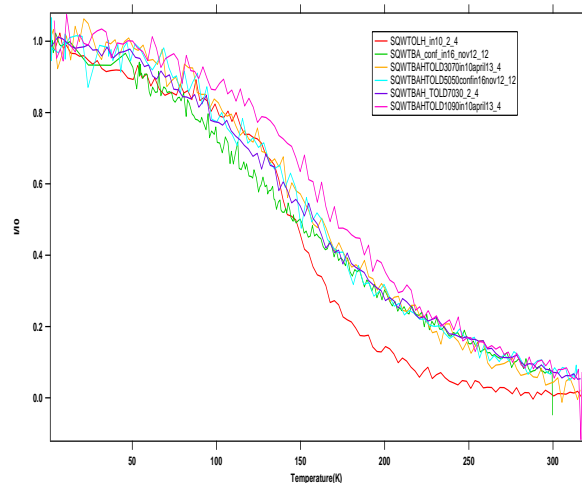


Fig.2. Fixed window elastic scans of different TBAH/TOLD mixtures confined in MCM-41.

Functional soft hybrid organic-inorganic nanomaterials: from macromolecular to self-assembled systems

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The main challenge to take up in the design of hybrid organic-inorganic materials is to keep the added value of inorganic entities while preventing their self-aggregation within the hybrid matrix. We will describe in this presentation the strategies we developed to design luminescent octahedral transition metal atom clusters containing hybrid nanomaterials.

The term "metal atom cluster" describes a finite group of metal atoms held together by metal-metal bonds. The $[(M_6L^i_8)L^a_6]^{n-}$ unit (a = apical, i = inner, M = Mo, Re; L = halogenide, chalcogenide, $1 < n < 8$) constitutes the basic building block in the octahedral cluster chemistry and is easily obtained *via* high temperature solid state synthesis. Metallic clusters show unusual electronic, magnetic and optical properties due to the full delocalization of valence electrons on the whole metallic scaffold. In particular, they can be highly emissive in the red-NIR area.

Two types of hybrid materials will be described: macromolecular and liquid crystalline (clustomesogen) materials. In both cases, inorganic clusters were introduced either by covalent grafting or by using supramolecular interactions (ionic self-assembling or host-guest strategies). We will show that whatever method is adopted, the transition metal cluster luminescence is kept and can sensitize the IR luminescence of trivalent rare earth ions.

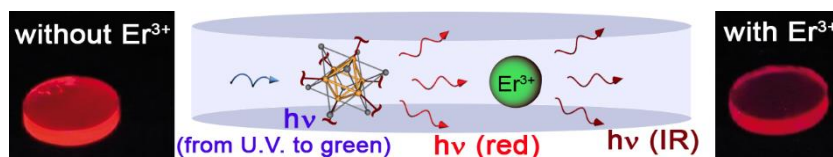


Figure 1: Polymer pellets containing Mo₆ clusters which sensitize Er³⁺ IR photoluminescence

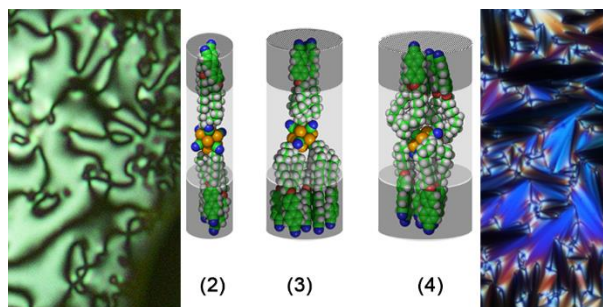


Figure 2: Polarized optical micrographs of nematogenic and smectogenic clustomesogens obtained via ionic assembling and their respective representation.

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Education

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Fields of Research

hybrid organic inorganic nanomaterials, polymers, liquid crystal, luminescence

Publications

1. "Tuned Red NIR phosphorescence of polyurethane hybrid composites embedding metallic nanoclusters for oxygen sensing.", M. Amela-Cortes, S. Paofai, S. Cordier, H. Folliot, Y. Molard, **Chem. Commun.**, **2015**, **51**, 8177-8180
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Supercritical Route for Green Materials

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Green materials processing is a philosophy of chemical research and engineering to encourage the design of products and processes that minimize the use and generation of hazardous substances, which involves 1) contribution of products to minimize environmental problems (CO₂ emission, environmental cleaning catalyst etc.), 2) recycle of materials to resources, 3) holistic life cycle assessment of the materials, and 4) combined multiple technological and operational systems for reduction of energy and resources. Supercritical fluids technology is expected to contribute for new materials synthesis with the green sustainable chemistry route, especially for nanomaterials.

So far, variety of materials have been developed, including ceramics, metals and polymers, but recent needs in the industries are of multi-functions of ceramics/metals and polymers. For fabricating multi-functional materials, we proposed a new method to synthesize organic modified nanoparticles (NPs) in supercritical water. Since the organic molecules and metal salt aqueous solutions are miscible under the supercritical state, and water molecule works as an acid/base catalyst for the reactions, organic-inorganic conjugate nanoparticles can be synthesized under the condition. This synthesis method can control the exposed surface of NPs, which shows high catalytic activity of nano-catalysis; This promotes the bitumen or biomass waste decomposition (endothermic reaction) at lower temperature without coke formation. This gives rise to recover the waste heat and the waste treatment problems at the same time, namely solve the energy (CO₂) problems.

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Supercritical Fluids, Nanoparticles

Publications

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Advanced nanostructured materials by design in supercritical fluids

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Cyril Aymonier is currently CNRS researcher at the “Institut de Chimie de la Matière Condensée de Bordeaux (ICMCB)”. He obtained his PhD in chemical engineering from University of Bordeaux (2000) where he focused on supercritical water oxidation of wastewater. He did a postdoctoral stay in Freiburg (2000-2002, Germany) with Pr R. Mülhaupt and Pr S. Mecking where he helped to develop novel approaches to design hybrid organic/inorganic nanoparticles. Now he is in charge of the department “Supercritical Fluids” of ICMCB (about 25 people). His current research interests are i) the study of the chemistry and nucleation & growth in supercritical fluids applied to the design of advanced nanostructured materials, ii) the study of materials recycling using supercritical fluids and iii) the development of the associated supercritical fluids based technologies. Cyril Aymonier has so far authored/co-authored 94 peer-reviewed journal articles, 6 book chapters and 15 patents. He was awarded by the CNRS bronze medal in 2011.



A strong collaboration exists with Pr Tadafumi Adschiri from WPI-AIMR (Tohoku University, Sendai) on the sustainable manufacturing of nanohybrid materials in the frame of the G8 Research Councils Initiative. This project allowed also developing interactions with the groups of Pr Masahiko Hirao and Pr Kohzo Itoh (University of Tokyo).

Abstract – The supercritical fluids method of advanced nanostructures manufacturing offers continuous, fast, scalable and sustainable routes towards high quality nanomaterials. Intermediate between solution based synthesis approaches and gas phase ones, the supercritical fluids route is a versatile method already been used to synthesize various highly crystalline inorganic materials (oxides, metals, nitrides, etc.) with a control of composition, size and morphology [1, 2].

The use of sc-water as main solvent is now extended to other fluids (alcohols, NH_3 , alkanes, ... and mixture of them) to synthesize nanostructures. This variety of solvents opens avenue towards the use of numerous precursors for the investigation of a very rich chemistry; this means the use of more complex systems with an increasing number of parameters. We propose to highlight the chemistry and nucleation & growth in supercritical water / alcohol applied to the synthesis of $\text{Ba}_x\text{Sr}_{1-x}\text{Ti}_y\text{Zr}_{1-y}\text{O}_3$ ($0 \leq x \leq 1$ - BST, $0 \leq y \leq 1$ - BTZ) [3]. The combination of *in situ* Synchrotron wide angle X-ray scattering (WAXS) with *ex situ* analyses as Fourier transform infrared spectroscopy (FTIR), Raman spectroscopy, X-ray photoelectron spectroscopy (XPS), X-ray diffraction (XRD) and high resolution transmission electron microscopy (HR-TEM) leads to a better understanding of the nanoparticle growth mechanism and so, to a better control of their physico-chemical properties. The densification of these unique BST, BTZ nanostructures by high pressure spark plasma sintering (SPS) conducts to the formation of reproducible and dense nanostructured ceramics with interesting ferroelectric properties [4]. However, the use of surfactants to control morphology and surface properties remains essential. Therefore, although sc-water is a solvent of choice, the poor water solubility of some surfactants could require other solvents systems such as alcohols, which could themselves behave as surface modifiers. The influence of 7 different alcohols – MeOH, EtOH, PrOH, iPrOH, ButOH,

PentOH and HexOH - in alcohothermal conditions (300 °C, 24.5 MPa) over CeO₂ nanocrystals (NCs) size, morphology and surface properties has been investigated. The crystallite size of the CeO₂ nanocrystals can be tuned in the range 3-7 nm depending on the considered alcohol, and their surface has been modified by these solvents without the use of surfactants. Mechanisms are proposed for the interaction of primary and secondary alcohols with CeO₂ surface and its functionalization during the synthesis [5, 6]. The understanding of the nucleation & growth of CeO₂ NCs in near- and supercritical alcohols is part of the collaboration with the group of Pr Adschiri [7]. The key role played by solvents will be also illustrated through the fast and continuous synthesis of GaN NCs in supercritical ammonia.

Finally, we propose to introduce the new methods we have developed coupling supercritical micro- and millifluidic for the design of advanced nanostructured materials [8]. Supercritical microfluidics was introduced few years ago to propose to improve the understanding and develop chemistries and processes for the design of advanced nanostructured materials through an access to *in situ* investigation and high screening capability [9]. As soon as the process is developed and the chemistry understood, the synthesis is made in millifluidic reactors to produce more materials for its characterization and its application. In this lecture, the interest of this original and efficient approach in Materials Science will be illustrated with the formation of exciton luminescent ZnO NCs, efficient Pd-based nanocatalysts with tailored surface properties and QDs with different morphologies [10, 11, 12].

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Dimensional crossover in coordination chemistry

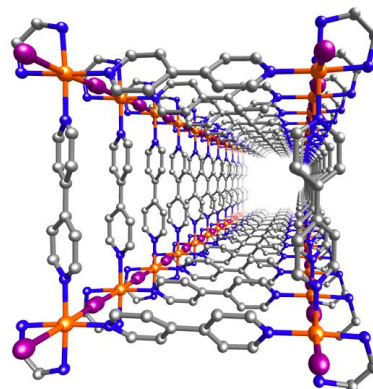
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Since the discovery of carbon nanotubes, they have attracted very wide scientific interest because of their characteristic electronic structure and conducting properties, and they have motivated the creation of many kinds of tubular nanomaterial. However, sometimes developing the structural and electronic tunings of nanotubes is subject to some potential limitations; for example, extreme synthetic conditions that mainly need high temperatures cause difficulties in the precise control of their size, shape and atomic constituents. Therefore, the fabrication of well-defined nanotubes with high tunability is a very challenging task. In contrast, the bottom-up approach for constructing nanostructures using metal-organic building blocks offers the advantage of controlling their size, shape, electronic states and also their robustness by substituting their structural components. Although many aspects of the physical and chemical properties of carbon nanotubes have been considered, those of metal-organic nanotubes have rarely been discussed so far.

Here, we demonstrate a bottom-up approach for the fabrication of well-defined dimensional-crossover nano-architectures with high tunability using metal ions and organic molecules as building blocks [1-4]. We succeeded in rationally constructing an assembly of square prism-shaped metal-organic nanotubes with aside of 2 nm. A uniform 1D channel is fabricated inside the tube, and H₂O and alcohol can be selectively adsorbed. Its optical gap is about 0.76 eV of semiconductive region, and X-ray and theoretical studies revealed its unique electronic structure of CDW quartets. In addition, its electronic states can be successively controlled by exchanges of structural components and guest molecules. The results presented here demonstrate a rational route to the creation of nanotubes with high tunabilities of structures and electronic states, and might also offer valuable insights into multifunctional nanomaterials.



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Publications

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Sensors and biosensors based on organic semiconductors

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Nowadays, diagnosis and continuous monitoring of physical, biochemical and chemical variables are of major interest because their possible changes or disruptions may cause adverse effects or even death. Among them, organic and inorganic chemicals control became of crucial importance due to their ubiquity in a wide variety of medical, agricultural and industrial applications. While the wide use of such chemicals has had significant economic and social benefits it has also led to the release of many micro-pollutants into the environment that are harmful even at very low concentration.

Therefore, an increased effort in fast and selective detection methods allowing real-time monitoring of their concentration changes is strongly necessary. For instance, chromatography techniques (high performance liquid chromatography (HPLC), liquid chromatography coupled with spectroscopy (LC-MS), gas chromatography (GC), capillary electrophoresis (CE) etc...) are methods extensively used for the determination of various chemicals disruptors. Although, these methods offer excellent selectivity and detection limits, they are not suitable for rapid processing of multiple samples and real-time detection. They involve highly trained operators, time-consuming detection processes, and complex pre-treatment steps requiring efficient low-cost alternatives.

These concerns have led to the development of emerging techniques with highly specific features. Thus, the design and fabrication of electrochemical and field effect transistors based sensors are both promising approaches for the future in diagnosis and monitoring. They fulfill the requirements in terms of selectivity, sensitivity, fabrication cost and size, as well as, in term of easiness of use.

In this context, we will present herein the preparation and the sensing properties of highly selective and specific sensors based on organic semiconductors [1].

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Publications

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Carrier injection and transport in organic and inorganic nano materials

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Flow of electrons and holes with charge, so called as carrier, is very important for electric conduction as well as for thermal conduction. Thermal conduction can also be available via phonon mediation, and both electric and thermal conduction in addition to spin momentum flow, play a very important role for energy conversion in materials science. In order to provide carriers into solid state materials, three types of methods can generally be employed: the first being replacement of elements in materials, the second being insertion of elements or molecules (intercalation process) into a space in a lattice, and the third is electric field induced effect generally used in field effect transistors (FETs). The former two are chemical approaches and the third is a physical one. In the first two categories, the approach by intercalation is of very importance especially in nano materials and organic materials since their ground states are generally categorized as the closed-shell electronic states and the carrier injection should be made without creating any large damage on their structure. The physical approach using transistor device structure, in the third classification, can be used both for organic and inorganic materials, where intriguingly the injection limit of carriers is remarkably different between inorganic and organic materials.

In this workshop, I will describe the present situation and understanding on the carrier injection and the transport in inorganic and organic materials, especially focusing on nano materials referring to our recent researches [1-5]. Followings are the topics to be presented in this workshop.

1. Carrier injection via intercalation process in inorganic and organic materials.
2. Carrier tuning and true electronic ground states in pure-carbon organic semiconductors.
3. Metal-semiconductor (MS) contact of transistor structure in inorganic and organic materials.

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Publications

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