



2<sup>nd</sup> World Conference on

# Industrial Chemistry and Water Treatment

May 22-23, 2017

Las Vegas, USA

# Keynote Forum

## Day 1

*Industrial Chemistry 2017*



## Masayoshi Tabata

Muroran Institute of Technology, Japan

### Emerging of stretched and contracted helices of substituted polyacetylenes and its molecular oscillation in solution

Stretched (cis-transoid) and contracted (cis-cisoid) helices of mono-substituted polyacetylenes (SPAs) were selectively prepared using a  $[\text{Rh}(\text{norbornadiene})\text{Cl}]_2$  in the presence of amine or alcohol cocatalyst in solution. The cis-transoid and cis-cisoid helices constructed from the aliphatic polyacetylenes ester main chain in solution showed an accordion-like helix oscillation and helios, respectively, where restricted rotations around the O-C bond in the ester side-chain are dynamically synchronized. The magnetic behavior of the cis and trans radicals of SPAs produced through the rotational scission of the C=C bonds is also reported.

#### Biography

Masayoshi Tabata has completed his PhD from Hokkaido University, Japan and Postdoctoral studies from United Kingdom and Sweden. After that he became Assistant Professor and Associated Professors at Hokkaido Univ., and Professor of Muroran Inst. of Tech., Japan. Moreover, he also became a senior research director at National Institute of Advanced Industrial Science & Tech. (AIST) Tsukuba, Japan, and Guest Professor at Paris Univ. in France.

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#### Notes:

# Industrial Chemistry and Water Treatment

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## Lidietta Giorno

*National Research Council, Italy*

### **Integrated membrane processes for sustainable industrial production and water treatment**

The increase of world population and the intensive demand for food, goods, water and energy is driving a depletion of resources as well as a dramatic impact on environment. It is clear that advanced technologies play a key role in providing strategies to face challenges of modern globalized society. Membrane technology is recognized among the most efficient, precise, flexible, clean, low energy input technology. Various nanostructured membrane-based processes are nowadays state-of-the-art in implementing separation at molecular level, recognition, concentration, conversion, formulation. Integrating different membrane operations as well as combining them with other type of technologies permits to efficiently tune output products and obtain co-products instead of byproducts or waste. For example, liquid beverage processing, active ingredients production, chemical manufacturing, biorefinery, safety, water treatment and water desalination well confirm these possibilities. Case studies will be illustrated concerning the development of integrated processes for the purification of vegetative water coming from olive oil industry with simultaneous recovery, transformation and formulation of biophenols based ingredients. The non-edible organic fraction could also be used to produce biogas and its suitable purification for energy use was achieved by using polymeric membranes. The achievements of membrane-based sea water desalination for both potable water production and minerals extraction will be highlighted. Membrane-based operations play a role also in monitoring and decontaminating air and water. An integrated system using biosensors are able to detect harmful gaseous substances and promote the activation of decontamination process based on enzyme-loaded membrane will be illustrated.

### **Biography**

Lidietta Giorno has her expertise in membrane science and technology. Her research activity include membrane bioengineering, biocatalytic membrane reactors, enzyme immobilization, nanostructured and multifunctional membranes, integrated membrane systems for bioseparations and bioconversions, downstream processing based on molecular separation, membrane chirotechnology, membrane emulsifier, integrated membrane operations for water treatment.

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### **Notes:**



## Jun-Ichi Kadokawa

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### Chemoenzymatic synthesis of polysaccharide-grafted polymeric materials

Biological macromolecules, such as polysaccharide and protein (peptide), are vital materials in living systems. Such functions are appeared by their controlled primary and higher-ordered structures. Furthermore, branched or grafted biological polymers are often appeared in nature and such complicated structures contribute to exhibiting important in vivo functions. Accordingly, synthetic method for combining several biological macromolecules into branching or grafting is expected to produce new functional polymers. On the basis of the viewpoint, we have reported the synthesis of amylose-grafted polymeric materials by chemoenzymatic approach, which is a combined method of phosphorylase, catalyzed enzymatic polymerization of  $\alpha$ -D-glucose 1-phosphate (G-1-P) monomer for the amylose production with appropriate chemical reactions. The phosphorylase-catalyzed enzymatic polymerization using G-1-P as a monomer proceeds with the construction of  $\alpha$ -glycosidic bond under mild conditions, leading to the direct formation of  $\alpha(1\rightarrow4)$ -glucan chain, i.e., amylose, in the aqueous media. To initiate the polymerization, a maltooligosaccharide is required as a primer in the initial reaction media. The synthesis of amylose-grafted heteropolysaccharides has been performed by combining the phosphorylase-catalyzed enzymatic polymerization with the appropriate chemical reaction (chemoenzymatic method). For example, amylose-grafted carboxymethyl cellulose (CMC) was synthesized as the following chemoenzymatic method. A maltooligosaccharide having an amino group was first introduced to the CMC by using condensing agent. Then, the phosphorylase-catalyzed enzymatic polymerization of G-1-P from the maltooligosaccharide chain ends on the product was performed to obtain the desired amylose-grafted CMC. The product had the rigid CMC main chain, which further assembled, leading to nanofibers by the formation of double helix between the long amylose graft chains in the intermolecular CMC chains. The chemoenzymatic synthesis of amylose-grafted poly  $\gamma$ -glutamic acid (PGA) as a new artificial polysaccharide-polypeptide conjugate was also investigated. The product formed a robust hydrogel, which could be converted into a regularly controlled porous material.

### Biography

Jun-Ichi Kadokawa holds PhD degree in Engineering. Currently, he is a Professor of Chemistry, Biotechnology and Chemical Engineering at Kagoshima University, Japan. He studied applied chemistry and materials chemistry at Tohoku University, where he received his MS degree in 1989 and PhD in 1992. He has then joined Yamagata University as a Research Associate. From 1996 to 1997, he has worked as a Visiting Scientist at the Max-Planck-Institute for Polymer Research in Germany. In 1999, he became an Associate Professor at Yamagata University and moved to Tohoku University in 2002. He was appointed as a Professor of Kagoshima University in 2004. His research interests focus on enzymatic synthesis of functional oligo- and polysaccharides and control of their higher-ordered structures. He has received the award for Encouragement of Research in Polymer Science (1997) and the Cellulose Society of Japan award (2009).

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### Notes:



## Majid Mohammadian

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### Numerical simulation of laterally confined vertical buoyant jets

In most cases, the density of wastewater effluents is less than that of the receiving water body. Therefore, the wastewater effluents are considered buoyant jet. A typical type of buoyant jets is the outfall of the wastewater treatment plants. In order to effectively design an outfall system, and minimize its environmental impact, the mixing mechanism of turbulent buoyant jets must be examined. It is essential to dispose the buoyant jets in a suitable condition, because these jets have dominant negative environmental impacts. In many cases, the effluent is bounded by limiting boundaries. This leads to a confined turbulent jet. The mixing characteristics of confined buoyant jets can be examined in different ways including experimental, numerical and theoretical methods. Limited studies in the literature are reported on numerical modeling of laterally confined vertical buoyant jets. In this paper, the mixing characteristics of a laterally confined vertical buoyant jet is studied using various turbulence models including the GGDH  $k-\epsilon$  turbulence model which is a buoyancy-corrected model. The numerical simulation results are compared to other models and experimental data experiments. The study demonstrates that GGDH  $k-\epsilon$  turbulence model improves the precision of simulations. It can thus be employed for examining the mixing characteristics of confined buoyant jets.

### Biography

Majid Mohammadian is an Associate Professor at the Department of Civil Engineering, who is an expert in the research field of the computational fluid dynamics. He is a former MIT Researcher and has also had two years of research experience at Environment Canada and New York University. He carries out research in the areas of numerical modeling in marine outfall systems, river engineering, environmental hydraulics, turbulence and computational methods. He is an Associate Editor of the *Journal of Applied Water Engineering and Research, Taylor and Francis (IAHR)*, Member of IAHR-IWA Leadership Committee on Marine Outfall Systems and was the Chair Person of the IAHR-IWA International Symposium on Outfall Systems (2016). The focus of his research is on marine outfall systems.

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### Notes:





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## Day 2

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## *Fumio Sanda*

*Kansai University, Japan*

### Precise synthesis of substituted polyacetylenes

Substituted polyacetylenes have received considerable attention, owing to their properties resulting from the  $\pi$ -conjugated backbone such as photoconductivity and electroluminescence. The introduction of functional groups at the side chains provides polyacetylenes with useful structural features including liquid crystallinity, molecular recognition, stimuli-responsiveness and gas permeability. Substituted polyacetylenes are synthesized by the polymerization of the corresponding acetylene monomers using transition-metal catalysts. Rh catalysts bearing a triphenylvinyl group polymerize substituted acetylene monomers in a living fashion to give polymers with controlled molecular weights, geometry and end structures. Pd catalysts bearing bulky phosphine ligands polymerize disubstituted acetylene monomers via the coordination-insertion mechanism. Substituted polyacetylenes bearing chiral substituents adopt helical conformations, whose predominant screw sense transforms between right and left-handed in  $\text{CHCl}_3/\text{MeOH}$  with respect to the solvent composition. The polymers prefer conformations with large dipole moments in polar media, confirmed by the semi empirical molecular orbital calculations, COSMO method.

### Biography

Fumio Sanda is a professor in Kansai University. His research studies includes Polymer Synthesis, Transition Metal Catalyzed Polymerization, Conjugated Polymers, Optically Active Polymers. He has received Nakamura award in the year 1997 and Award of Japan Thermosetting Plastics in 2014 and many more

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### Notes:



## Hyoyoung Lee

Sungkyunkwan University, South Korea

### Crystalline/amorphous low energy bandgap TiO<sub>2</sub> materials prepared in solution and their industrial applications

Recently, surface-disordered TiO<sub>2</sub>, referred to as black TiO<sub>2</sub>, which can absorb both visible and near-infrared solar light that has triggered an explosion of interest in many important applications. Here, we demonstrate a selective reduction of commercialized degussa P-25 TiO<sub>2</sub> nanoparticles using simple room-temperature solution processing, which maintains the unique three-phase interfaces composed of ordered white-anatase and disordered black-rutile with open structures for easy electrolyte access. The strong reducing agent in superbase, which consists of lithium ion ethylenediamine (Li-EDA), can disorder only the white-rutile phase of P-25. Single P-25 TiO<sub>2</sub> nanoparticles with this engineered surface made immediate contact with the electrolyte. This contact is called white-black-electrolyte three-phase interfaces and can not only efficiently internally separate electrons/holes through type-II bandgap alignment but also induce a strong hydrogen (H<sub>2</sub>) evolution surface reaction. The white-black-electrolyte three-phase interfaces exhibited outstanding H<sub>2</sub> production rates of 13.89 mmol/h/g using 0.5 wt.% Pt (co-catalyst) and 3.46 mmol/h/g without using any co-catalyst. These values are the highest recorded in the world to date. In addition, our newly developed crystalline/amorphous reduced TiO<sub>2</sub> (rTiO<sub>2</sub>) that has low energy bandgap can effectively generate reactive oxygen species (ROS) under solar light and successfully remove a bloom of algae. Only reduced TiO<sub>2</sub> materials can generate ROS under solar light, which was confirmed by electron spin resonance. Among the three different types of Li-EDA treated TiO<sub>2</sub> (anatase, rutile and both phased TiO<sub>2</sub>), the both phased rTiO<sub>2</sub> showed the best performance to produce ROS. The generated ROS effectively removed the common green algae *Chlamydomonas*. This is the first report on algae degradation under solar light, proving the feasibility of commercially available products for disinfection. Finally, we like to introduce transition metal chalcogenide materials for the hydrogen evolution reaction and energy storage with graphene flakes.

#### Biography

Hyoyoung Lee has received his PhD degree at Department of Chemistry, University of Mississippi (USA) in 1997. He did his Post-doctorate at North Carolina State University, USA, for 2 years. He has worked at Electronics and Telecommunications Research Institute from 2000 to 2009 as a Team Leader. He moved to Sungkyunkwan University and has served as a Full Professor at Department of Chemistry, lecturing Organic Chemistry. He has served as a Director of National Creative Research Initiatives (NCRI), Center of Smart Molecular Memory from 2006 to 2015. Currently, he has serving as an Associate Director of Centre for Integrated Nanostructure Physics (CINAP), Institute of Basic Science (IBS) from November 2015. His current research area is on organic semiconducting materials including low bandgap TiO<sub>2</sub> and devices including molecular/organic memory, OLED, OTFT, sensors, Energy harvesting and storage, graphene oxide, reduced graphene oxide and 2D transition metal chalcogenide (TMC). He has written more than 120 journal articles with top-tier journals.

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#### Notes:





## Toshiki Aoki

Niigata University, Japan

### Unusual phenomena in helix-sense-selective polymerization and its product

In 1993, we accidentally discovered the first example of an asymmetric-induced polymerization (AIP) of chiral substituted acetylene, during our study on optical resolution membranes. Since poly substituted acetylenes have no asymmetric carbons, the optical activity is caused by the one-handed helical conformation. Therefore, the optical activity is often not static but dynamic. In 2003, we reported the first helix-sense-selective polymerization (HSSP) of an achiral substituted acetylene by using a chiral catalytic system consisting of chiral phenyl ethylamine (PEA) and a rhodium dimer complex ( $[\text{Rh}(\text{nbd})\text{Cl}]_2$ , nbd=2,5-norbornadiene). The achiral monomer had two hydroxymethyl groups and a relatively hydrophobic substituent and the one-handed helicity of the resulting polymer was statically maintained by intramolecular hydrogen bonds in nonpolar solvents. After the discovery, we found some new monomers suitable for the HSSP reaction and have tried to control the polymerization. During these studies, some unusual phenomena were also found to occur in the HSSP process. We found that the HSSP of achiral phenylacetylenes having two hydroxy groups was catalyzed by the chiral polymers prepared by the HSSP of the same or similar achiral phenylacetylenes instead of using the chiral cocatalyst like PEA (Self-HSSP). In addition, it shows the possibility of in-situ self-catalyzed HSSP where the HSSP products formed during the HSSP functioned in-situ as a chiral cocatalyst for the HSSP of the same monomer (In-situ self-HSSP). In addition to the discovery of self-HSSP, other several unusual phenomena were observed in the HSSP of RDHPA. For example, the sense of the helicity of the polymers prepared by HSSP was controlled by changing non-chiral conditions such as the molar ratio of the chiral cocatalyst to the rhodium complex (Reversal HSSP). That may be caused by formation of different chiral rhodium species depending on the ratio. In addition, HSSP was also realized without any chiral source (Spontaneous HSSP). It may result from the formation of a chiral supramolecular compound of the monomer. Since the polymer resulting from HSSP adopts very tight cis-cisoidal conformation and therefore a rigid rod structure, which is not seen in any other poly (substituted acetylenes), it shows many unusual and interesting properties, including unique types of reactivity. For example, in 2013, we reported highly selective photo aromatization (SCAT) of the very tight cis-cisoidal polymer prepared by HSSP.

### Biography

Toshiki Aoki has received his Doctorate degree (1987) on synthesis and oxygen permeability of graft copolymers from oligosiloxane macromonomers in Department of Applied Chemistry at Nagoya University, Japan. He has joined Fluorine Chemistry Division at Government Industrial Research Institute, Nagoya in 1987-1989. He has then moved to Department of Applied Chemistry at Niigata University in 1989. He has worked at Niigata University as an Assistant Professor (1989), Associate Professor (1995) and Full Professor (2000). He has worked as a Visiting Scientist at University of Southern California from 1998-1999. His research interest covers synthesis of functional polymers, including synthesis of new chiral polymers for permselective membranes. His recent interest is in synthesis and application of two-dimensional polymers using HSSP and SCAT reactions.

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### Notes:

## Industrial Chemistry and Water Treatment

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## Dhanesh Chandra

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### Hydrogen technology for automobiles in the 21<sup>st</sup> century towards more secure and cleaner environment

Hydrogen is expected to play an important role in future energy scenarios, as it could resolve growing concerns about world's energy supply, security, air pollution, and greenhouse gas (GHG) emissions. Hydrogen production from renewable resources can potentially reduce the CO<sub>2</sub> emissions. Hydrogen is a non-toxic, clean energy carrier that has high specific energy on a mass basis (e.g., the energy content of 9.5 kg of hydrogen is equivalent to that of 25 kg of gasoline). Worldwide H<sub>2</sub> production is ~ 500 billion.m<sup>3</sup> annually with ~6.5 EJ (1EJ=109 GJ) of energy. The exhaust from the H<sub>2</sub> vehicles is water. Early developments (from 1960) were focused on H<sub>2</sub>-IC engine vehicles. In 2001, BMW introduced H<sub>2</sub>-IC engine vehicles. Significant advancements in fuel cell technologies and initiatives offered by the US DOE, world-wide governmental agencies, and industries led to the development of prototypes H<sub>2</sub>-fuel cell electric automobiles. In the last 10-15 years many auto manufacturers, including Toyota, Honda, Hyundai, Ford, General Motors, Daimler Chrysler and others have developed fuel cell vehicles, some are already becoming commercial. Many countries are installing hydrogen fueling stations but they are relatively few clustered around big, highly populated cities. Low pressure, solid state metal hydrides, such as LaNi<sub>4.8</sub>Sn<sub>0.2</sub>, have already been developed for space applications, but they are very heavy and have low gravimetric hydrogen density of ~2 wt.% for vehicular applications. Light weight and low pressure (LP) complex hydrides, such as Mg(BH<sub>4</sub>)<sub>2</sub>, Li<sub>2</sub>NH-LiNH<sub>2</sub> and other light weight systems with ~10 to 18 wt.% H capacity are still in developmental stages. Non withstanding the LP solid state systems, Toyota and other manufacturers started using high pressure (~700 bar) H<sub>2</sub>, carbon fiber composite, cylinders which appear to be functional in the latest vehicles under normal operations. The H<sub>2</sub> based vehicular technological developments, and challenges associated with this technology will be presented.

#### Biography

Dhanesh Chandra is a Foundation Professor of Materials Science and Engineering in the College of Engineering at the University of Nevada Reno, USA. He has over 100 scientific publications and is a Member of Hydrogen IEA-Task 32. He wrote a book chapter: *Intermetallics* for Hydrogen Storage edited by G Walker, Woodhead Publishing (2008).

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#### Notes:

## *Yasuteru Mawatari*

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### **Color gradation of substituted polyacetylenes: Molecular design, synthesis, and characterization of their helical structures**

Main-chains in substituted polyacetylenes (SPAs) are twisted into a helical structure in order to avoid steric hindrances between neighboring side-chains. We have previously demonstrated that the color of SPAs having phenyl rings, called poly(arylacetylene)s (PAAs) strongly depended on molecular structure of the side-chains in their aromatic ring and on solvents using by the polymerization reaction. In this work, we focused on relationship between color of PAAs and their helical structures. Designed PAAs having phenyl or naphthyl rings were synthesized and characterized to elucidate precise helical structures containing degree of twist and distance of aromatic rings in side-chains

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