YNU 横浜国立大学
YOKOHAMA National University

Japan-India YNU Symposium 2017

"Emerging Materials & Systems for Green and Life Innovations"

Co-organized with
GMI Symposium 2017 "Nano-materials for Green Applications"

Jointly organized with
YEIS International Forum 2017

Program

Japan-India YNU Symposium 2017

"Emerging Materials & Systems for Green and Life Innovations"

Co-organized with

GMI Symposium 2017 "Nano-materials for Green Applications"

Jointly organized with

YEIS International Forum 2017

Contents

Emergency Contact

Assoc. Prof. Kazuho Nakamura
Tel: 045-339-3980
Mobile: 090-4618-8858
E-mail: naka1@ynu.ac.jp

Preface

Welcome to YNU & Yokohama!

It is a great pleasure for us to hold the first YNU Symposium at Yokohama with a theme of Emerging Materials & Systems for Green and Life Innovations. Green and Life Innovations have been at the forefront of the Japanese research initiatives in the 21st century. Environment and Health are the two important global topics of research considering that the world is facing serious challenges in both issues. Under these circumstances and realizing the growing importance of India-Japan partnership in science and technology, the first YNU Symposium is organized to develop stronger collaboration among Indian and Japanese researchers in both countries, especially CBIC (Chennai-Bangalore Industrial Corridor) and Yokohama.

This symposium consists in scientific lectures on these topics, posters by YNU students, and pre & post-events. We hope you will enjoy this YNU Symposium and communicate with new friends from attendees from YNU and colleagues. We also expect this program will contribute to the further collaboration between India and Japan.

Meguru Kaminoyama

Prof. Meguru Kaminoyama
Faculty of Engineering
Yokohama National University
Yokohama, Japan

Schedule at a Glance

	Tokiwadai campus @YNU	Yokohama Symposia @Sangyo Boeki Center Building 9F			Minato mirai campus @YNU
	Dec. 12 (Tue)	Dec. 13 (Wed)	Dec. 14 (Thu)	Dec. 15 (Fri)	
9:00	Visit to YNU	Registration	Prof. Dr. Katsunori Okajima	Company Visit and Excursion	Assoc. Prof. Dr. Katsunari Yoshioka
9:20			Asst. Prof. Dr. Thakerng Wongsirichot		Assoc. Prof. Dr. Takashi Tomii
9:40		Opening Prof. A. Kannan	Asst. Prof. Dr. Wannarat Suntiamorntut		Discussion
10:00			Assoc. Prof. Dr. Shushi Harashita		
10:20		Dr. Swadhin K. Behera	Asst. Prof. Dr. Supawadee Prugsapitak		
10:40		Assoc. Prof. Mahesh Ganesapillai	Asst. Prof. Dr. Sakuna Charoenpanyasak		
11:00		Assoc. Prof. Aruna Singh	Prof. Gautam Biswas		
11:20		Assoc. Prof. Kazuho Nakamura			
11:40		Lunch	Prof. D. Mohan		
12:00	Lunch		Lunch		
12:20					
12:40		Prof. K Ganapathy Ayappa	Prof. N. Rajendran		
13:00	Visit to YNU				
13:20		Prof. Fumihiro Wakai	Prof. Yoshihiro Kubota		
13:40		Assoc. Prof. Raghuram Chetty	Prof. Osamu Takai		
14:00		Assoc. Prof. Abhishek Singh	Prof. Gautam Biswas		
14:20		Prof. Kaoru Ohno	Mr. Jungo Kawagoe		
14:40		Assist. Prof. Ashutosh Kumar Dubey	Mr. Takeo TANAKA Dr. Fumihiro Haga		
15:00	Free	Assoc. Prof. B. Venkata Manoj Kumar	Dr. Kenji.Yao JICA		
15:20		Break	Break Vice Chencellor, Dr.M.BHASKARAN		
15:40		Asst. Prof. Dr. Amnart Pohthong			
16:00		Lec. Dr. Shinichi Shirakawa	Asscoc. Prof. Ayyamperumal Sakthivel		
16:20		Dr. Tanwa Arpornthip	Prof. Rajib Bandyopadhyay		
16:40		Lec. Dr. Erika Ushikoshi	Dr. Thirumalaiswamy Raja		
17:00		Poster (Core time)	Assoc. Prof. Yoshiyuki Kuroda		
17:20			Prof. Yoshitake		
17:40		Free	Closing Move to JICA Yokohama		
18:00					
18:20					
18:40					
19:00			Party	Dinner	
19:20					
19:40					

Japan-India YNU Symposium 2017 **GMI Symposium 2017** **YEIS International Forum 2017**

Joint Symposium Program

December 13 (Wed), 2017

Venue: **"Yokohama Symposia" (Sangyo Boeki Center Building 9F)**

9:10		**Registration**
9:30		**Opening** **Welcome Address** Chair: Prof. Hideaki Yoshitake Prof. Meguru Kaminoyama Prof. Yoshihiro Kubota Prof. Seiya Negami

Session 1 : Japan-India YNU Symposium 2017

Chair: N. Rajendran, A. Suzuki

9:50	01-JI-01	Treatment of Aqueous Wastes Through Wind and Solar Energy Aided Evaporation Kannan Aravamudan Indian Institute of Technology Madras, India
10:20	02-JI-02	Developing climate applications for sustainable future Swadhin Behera JAMSTEC, Japan
10:50	03-JI-03	Potential of Value Generating Toilet Systems Mahesh Ganesapillai VIT University, India
11:10	04-JI-04	Integrated systems to treat Municipal solid waste (MSW) - An Indian Scenario Aruna Singh VIT University, India
11:30	05-JI-05	Fouling Phenomena in Membrane Filtration and Design of Filters Kazuho Nakamura Yokohama National University, Japan
11:50		**LUNCH and BREAK**

Session 2 : Japan-India YNU Symposium 2017

Chair: D. Mohan, H. Yoshitake

12:50	06-JI-06	Adsorbed Natural Gas for Onboard Storage: Tailoring Materials, Challenges and Perspective K. G. Ayappa Indian Institute of Science, India
13:20	07-JI-07	Microscopic Sintering Forces behind Macroscopic Continuum Theory of Sintering F. Wakai Tokyo Institute of Technology, Japan
13:50	08-JI-08	Shape Controlled Nanostructures for Electrocatalytic Applications Raghuram Chetty Indian Institute of Technology Madras, India
14:10	09-JI-09	Machine-Learning Assisted Accurate Band Gap Predictions of Functionalized MXene Abhishek K. Singh Indian Institute of Science, India
14:30	10-JI-10	Production of Li+@C60 Kaoru Ohno Yokohama National University, Japan
14:50	11-JI-11	Biocompatible Ferroelectrics as a New Generation Implants for Biomedical Applications Ashutosh Kumar Dubey Indian Institute of Technology (BHU), India
15:10	12-JI-12	Surface and subsurface studies of worn SiC based composites for green transport engines systems B. Venkata Manoj Kumar Indian Institute of Technology Roorkee, India
15:30		**BREAK**

Session 3 : YEIS International Forum 2017

Chair: K. Matsui

15:40 13-YEIS-01 The adoption of early test-case generation
Amnart Pohthong
Prince of Songkla University, Thailand

16:00 14-YEIS-02 On the optimization of deep neural network architectures
Shinichi Shirakawa
Yokohama National University, Japan

16:20 15-YEIS-03 Integrated water information management
Tanwa Arpornthip
Prince of Songkla University, Thailand

16:40 16-YEIS-04 Domain perturbation problem for the Stokes equations
Erika Ushikoshi
Yokohama National University, Japan

Poster Presentation

December 13 (Wed), 2017
Venue: Reception Space at "Yokohama Symposia"

Chair: K. Aramaki, M. Iijima

17:00-17:40

PO-01 Growth of microstructures in Ni-Al alloy from first principles based phase field method"
Swastibrata Bhattacharyya, Ryoji Sahara and Kaoru Ohno
Yokohama National University, Japan

PO-02 Reaction between α, β-unsaturated aldehyde and alcohol on gold supported on nanostructured zirconia
Satoru Nakahara, Hideaki Yoshitake
Yokohama National University, Japan

PO-03 Polymerization of functionalized silica nanoparticles
Keisuke Fukuda, Hideaki Yoshitake
Yokohama National University, Japan

PO-04 Synthetic investigation of new zeolite YNU-5"
Naoto Nakazawa, Yuka Yoshida, Satoshi Inagaki, Yoshihiro Kubota
Yokohama National University, Japan

PO-05 Catalytic performance of Ce-modified MCM-68 zeolite in the dimethyl ether-to-olefin reaction
Qiao Han, Kizuku Enoeda, Satoshi Inagaki, Yoshihiro Kubota
Yokohama National University, Japan

PO-06 The analysis of oxygen dissolution into water via membrane contactor
Yuji Arai, Kazuho Nakamura
Yokohama National University, Japan

PO-07 Effect of MF treatment of mother liquor on MSZW in cooling crystallization of L-glutamic acid
Shimizu Yosuke, Kazuho Nakamura
Yokohama National University, Japan

PO-08 Emulsion-based gels with thermally switchable transparency
Ryosuke Horie
Yokohama National University, Japan

PO-09 Effect of PEI-oleic acid complex structures on in-situ solidification properties of Si3N4/α-terpineol dense slurry induced by addition of multifunctional acrylates
Kenta Hasegawa, Motoyuki Iijima, Junichi Tatami
Yokohama National University, Japan

PO-10 Fabrication of porous TiN structures from TiO2 colloids using polymer monolith as a template
Atsushi Uga, Motoyuki Iijima, Junichi Tatami
Yokohama National University, Japan

PO-11 Prediction of strength of a ceramic sintered body by three dimensional observation using optical coherence tomography
FumikaSakamoto[1], Takuma Takahashi[2], Junichi Tatami[1,2], Motoyuki Iijima[1,2]
1 Yokohama National University, Japan
2 Kanagawa Industrial Institute of Science and Technology, Japan

PO-12 Control of sintering behavior of NiO/GDC porous ceramics by mechanical treatment of raw materials
Kajii Kenji[1], Junichi Tatami[1,2], Motoyuki Iijima[1,2], Takuma Takahashi[2]
1 Yokohama National University, Japan
2 Kanagawa Industrial Institute of Science and Technology, Japan

PO-13 Grain boundary strength of porous SiC measured by microcantilever beam technique
Yumi Imoto[1], Junichi Tatami[1,2], Motoyuki Iijima[1,2], Takuma Takahashi[2], Tsukaho Yahagi[2]
1 Yokohama National University, Japan
2 Kanagawa Industrial Institute of Science and Technology, Japan

PO-14 One-step formulation of nonionic surfactant bicelles(NSBs) by a bouble-tailed polyglycerol-type nonionic surfactant
Chikahiro Iwata
Yokohama National University, Japan

PO-15 Oxygen supply and oxidative stress in pancreatic β-cell spheroids
Dina Myasnikova, Junji Fukuda
Yokohama National University, Japan

PO-16 Fabrication of double layered vascular structure
Shimazu Yuka[1], Zhilian Yue[2], Gordon Wallace[2], Junji Fukuda[1]
1.Yokohama National University, Japan, 2. University of Wollongong, IPRI

PO-17 Estimation by image analysis of time evolution of the crystal particle aggregation state during batch cooling crystallization
H. Hayashi, R. Misumi, M. Kaminoyama
Yokohama National University, Japan

PO-18 Effects of operational conditions on flow behaviour and drop size distributions in an annular centrifugal contactor
S. Okamoto, R. Misumi, M. Kaminoyama
Yokohama National University, Japan

PO-19 Effects of peel angle on peel force of adhesive tape from soft adherend
Yoshiki Sugizaki, Ryo Ichikawa and Atsushi Suzuki
Yokohama National University, Japan

PO-20 Development of high-strength poly(vinyl alcohol) hydrogels by unidirectional freezing methods
Shun Nakamura and Atsushi Suzuki
Yokohama National University, Japan

PO-21 Estimation of gestures for utterance text using neural network
Eiichi Asakawa
Yokohama National University, Japan

PO-22 Image simulation and perception model of aged color objects
Atsushi Moriwaki
Yokohama National University, Japan

PO-23 Variations of colorings of graphs in topological graph theory
Masayuki Fujita, Yumiko Ohno
Yokohama National University, Japan

PO-24 Automorphism groups of superspecial curves of genus 4 over F11
Hayato Senda
Yokohama National University, Japan

PO-25 ECOLOG: A database of EV energy consumption log acquired by vehicle mounted sensors
Toshiaki Uemura
Yokohama National University, Japan

PO-26 SandPrint: Gathering intelligence against malware sandbox evasion
Wataru Ueno, Rui Tanabe
Yokohama National University, Japan

December 14 (Thu), 2017

Venue: **“Yokohama Symposia” (Sangyo Boeki Center Building 9F)**

Session 4 : YEIS International Forum 2017
Chair: T. Yamada

9:10	17-YEIS-05	Crossmodal study on food perception with Augmented Reality Katsunori Okajima Yokohama National University, Japan
9:30	18-YEIS-06	A mobile application for biliary atresia detection in children using image processing and data mining techniques Thakerng Wongsirichot Prince of Songkla University, Thailand
9:50	19-YEIS-07	Smart connected communities in Smart City: Phuket City (case study) Wannarat Suntiamorntut Prince of Songkla University, Thailand
10:10	20-YEIS-08	Superspecial curves of genus 4 over small finite fields Shushi Harashita Yokohama National University, Japan
10:30	21-YEIS-09	On some Diophantine equations over complex quadratic number fields Supawadee Prugsapitak Prince of Songkla University, Thailand
10:50	22-YEIS-10	Tracking system based on IoT: Smart City Sakuna Charoenpanyasak Prince of Songkla University, Thailand

Session 5 : Japan-India YNU Symposium 2017
Chair: A. Kannan, K. Nishino

11:10	23-JI-13	Bubble entrapment during liquid drop impact on liquid pool Gautam Biswas Indian Institute of Technology Guwahati, India
11:40	24-JI-14	Advanced Materials for Membranes for Cleaner Environment D. Mohan Hindustan Institute of Technology and Science, India
12:00		**LUNCH and BREAK**

Session 6 : Japan-India YNU Symposium 2017

Chair: K Ganapathy Ayappa, J. Tatami

12:50 25-JI-15 Development of titania nanotubes for drug delivery applications
N. Rajendran
Anna University, India

13:20 26-JI-16 Zeolite-Based Nanoporous Materials as High-Performance Catalysts
Yoshihiro Kubota
Yokohama National University, Japan

13:50 27-JI-17 Surface Modification by Fine Bubble Low Ozonated Water (Fblow®) for Plating on Plastics
Osamu Takai
Kanto Gakuin University, Japan

Session 7 : Japan-India YNU Symposium 2017

Chair: *K. Nakamura*

14:10 28-JI-18 Introduction of IIT Guwahati and Collaboration with YNU
Gautam Biswas
Indian Institute of Technology Guwahati, India

14:30 29-JI-19 International Expansion of Sewage Works in Yokohama
Jungo Kawagoe
Environmental Planning Bureau City of Yokohama

14:40 30-JI-20 Water resource conservation and Non-revenue Water reduction
Takeo Tanaka
Yokohama Waterworks Bureau City of Yokohama

14:50 31-JI-21 Nissan Research Activity in India
Fumihiro Haga
Nissan Motor Co., Ltd.

15:00 32-JI-22 FX's New Cellulosic Plastic Technology
Kenji.Yao
Fuji Xerox

15:10 33-JI-23 JICA
Takahiro Ikenoue
Japan International Cooperation Agency

15:20 **BREAK**

Session 8 : GMI Symposium 2017

Chair: Y. Kubota

15:30 34-GMI-01 Eco-friendly Seed and Crop Fortification Techniques to Augment Biodynamic Farming Systems
M. Bhaskaran
Tamil Nadu Open University, India

16:00 35-GMI-02 Composite and Functional Silico-aluminophosphate Based Materials: Preparation, Characterization and Its Catalytic Applications
Ayyamperumal Sakthivel
Central University of Kerala, India

16:20 36-GMI-03 Porous Catalytic Materials for Biodiesel Production
Rajib Bandyopadhyay
Pandit Deendayal Petroleum University, India

16:40 37-GMI-04 Role of CO_2 as a Soft Oxidant for Oxidative Dehydrogenation Reaction of Lower Hydrocarbons Over Mixed Metal Oxide Catalysts
Thirumalaiswamy Raja
CSIR-NCL, India

17:00 38-GMI-05 Chemical Design of Layered Double Hydroxide Nanoparticles for Water Purification
Yoshiyuki Kuroda
Yokohama National University, Japan.

17:20 39-GMI-06 Selectivities in Adsorptions Induced by Surface Curvature of Functionalized Mesostructured Silica
Hideaki Yoshitake
Yokohama National University, Japan

17:40 **Closing Remarks**

19:00-21:00 **Party @ JICA Yokohama**

Abstracts

Treatment of Aqueous Wastes Through Wind and Solar Energy Aided Evaporation

Kannan Aravamudan[1], Ligy Philip[2], S. Murti Bhallamudi[2], K. S. Reddy[3]

[1] Department of Chemical Engineering, [2] Department of Civil Engineering, [3] Department of Mechanical Engineering, Indian Institute of Technology Madras, Chennai 600036

kannan@iitm.ac.in

Strict norms such as zero-discharge stipulated by pollution control boards have led to installation of common effluent treatment plants in several textile and dyeing industrial clusters. The effluents after treatment in several units are handled in reverse osmosis (RO) units to produce rich brine. The rich brine is further evaporated typically by solar/mechanical means, followed by chilling and crystallization to finally recover the solids. Direct solar and mechanical evaporation means are beset by poor performance and high fuel costs [1]. The present study describes an environmentally friendly and economical waste management strategy aided by solar energy, wind and enhanced surface area evaporation. The concentration tower is a packed framework irrigated with concentrated brine and is based on the concept of Gradierwerk found in German health resorts [2].

Experimental investigations revealed that preheating the water by solar energy increased evaporation rates. The evaporation rates were also influenced by concentration of the brine, relative humidity of the air and material, geometry as well as configurations of the packing employed. The evaporation process in the tower was simulated using a mathematical model developed from first principles [3]. The field data collected typically over 18 hours of daily operation were used to estimate the Number of Transfer Units (NTU) that may be used as a measure of tower capability for evaporation. This process holds considerable promise in dry windy places for RO reject management. Simulations enabled quick design and performance analysis of this scheme.

References

[1] L. Philp, K. S. Reddy, B. Kumar, S. M. Bhallamudi, A. Kannan, *Desal.* 2013, 317, 1.

[2] A. Graczykowska-Koczorowska, K. Marciniak, I. Ponikowska, *Z. Physiother.* 1978, 30, 300.

[3] K. Aravamudan, V. Harikumar, B. Kumar, L. Philip, S. M. Bhallamudi, K. S. Reddy, *Desal.* 2014, 340, 18.

Acknowledgements:

This research was supported by the Department of Environment and Forest, Tamil Nadu, India. The authors also acknowledge the Tamil Nadu Pollution Control Board, Green Textile Movement (GTM), Tamil Nadu and Free Look Fashions, Plot No. R7, State Industries

Promotion Corporation of Tamil Nadu (SIPCOT), Perundurai, Erode (Dist.), Tamil Nadu for all the help provided.

Biography

Dr. Kannan Aravamudan
Professor and Head, Department of Chemical Engineering
Indian Institute of Technology Madras, Chennai – 600036
INDIA

Educational background

B. Tech. (Anna University, 1988), M. Tech. (IIT Madras, 1990), Ph.D. (McMaster University, Canada, 1995)

Engineer (R&D Centre, Engineers India Limited, Haryana, India, 1990), Executive (Technology Innovation Centre, Larsen & Toubro, Baroda, 1995-1996), Assistant Professor (IIT Kanpur, 1996-1998, IIT Madras 1998-2006), Associate Professor (IIT Madras, 2006-2010), Professor (IIT Madras, 2010-current)

Academic Highlights/ Major Achievements/ Awards

P&T Scholarship for academic performance, Mico Bosch award for best M. Tech. Project, McMaster CIDA scholarship for academics, Shell Canada Award for Research Excellence, INAE Young Engineer Award for contributions to Mass Transfer, AICTE Career Award for Young Teachers

Present Research Interests: Process Intensification, Environmental Pollution Control, Process Modeling, Simulation and Optimization for Reaction and Transport Processes, Statistical Design of Experiments for analysis of engines to minimize emission of pollutants.

Contact E-mail: kannan@iitm.ac.in

Developing climate applications for sustainable future

Swadhin Behera, Takeshi Doi, Yushi Morioka, J.V. Ratnam and Takayoshi Ikeda

Application Laboratory, JAMSTEC, Yokohama, Japan

behera@jamstec.go.jp

Climate variations play a big role in the socio-economic conditions of the highly populated Asian region. Besides the seasonal monsoons, ocean-atmosphere coupled variations El Nino and El Nino Modoki phenomena in the tropical Pacific Ocean and the Indian Ocean dipole (IOD) phenomenon in the tropical Indian Ocean are the dominant modes of climate variations that influence the regional economies. Therefore, it is important to develop accurate prediction systems for those phenomena and predication based climate applications for the sustainable developments of the region. At JAMSTEC, we have been developing an ocean-atmosphere coupled model called the SINTEX-F for accurate predictions of El Nino and IOD variations. The model predicts the El Nino one year to two years ahead and the IOD several seasons ahead with great accuracy. Therefore, the model is considered as the leading model in the world for the prediction of El Nino, El Nino Modoki and IOD and experimental predictions are conducted every month using the model.

In order to further improve the accuracy and realize prediction in a wider area, we are conducting research on the understanding and predicting the underlying processes. The prediction skills are evaluated and the accuracy of the predictions is improved by further fine-tuning of the models. In addition to investigating tropical phenomena such as the El Niño, we are also studying El Niño-like phenomenon occurring on the eastern coasts of the oceans called coastal Niño.

In order to apply our climate predictions for the benefit of the society and to make full use of the large amount of ensemble predictions, we are developing information dissemination methods based on artificial intelligence and machine learning methods. The prediction information is applied in the studies of crop yield (through a project based on environmental research promotion funding). In another project, under the SATREPS framework, an early warning system for malaria incidences in South Africa is being developed in collaboration with Tropical Medical Research Institute of Nagasaki University. We are also developing heatwave early warning systems based on the analysis results of heatwaves (Fig. 1) in India[1] and neighboring countries. By conducting experimental seasonal forecasts and verifying their accuracy through these societal applications, we hope to improve forecast accuracies and contribute to the goals of the sustainable developments of the regional societies.

References

[1] J. V. Ratnam, S. K. Behera, S. B. Ratna, M. Rajeevan & T. Yamagata, 2016: Anatomy of Indian heatwaves, *Scientific Reports, 6, 24395, doi:10.1038/srep24395*

Acknowledgements:

This research was partly carried out for the iDEWS project supported by SATREPS Program of JICA/AMED in Japan and ACCESS (NRF/DST) in South Africa.

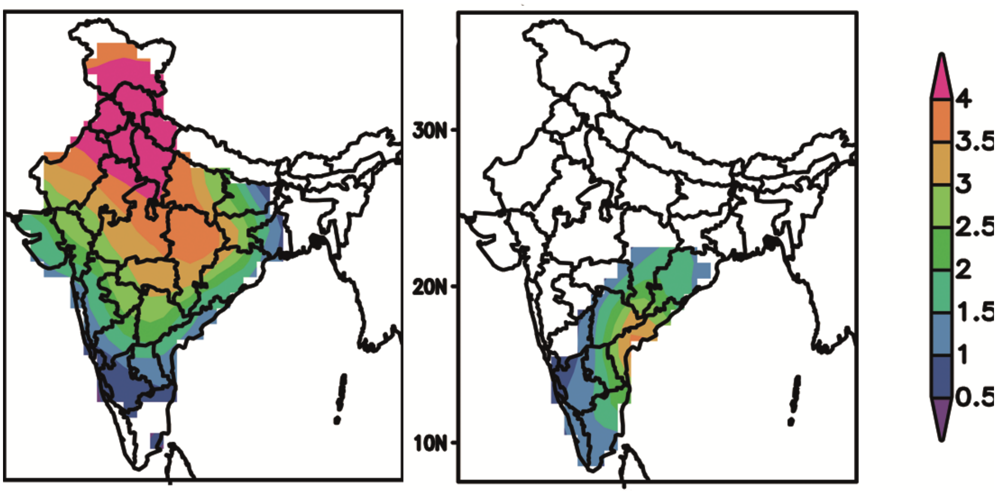


Figure 1. Composites of surface temperatures (^{0}C) associated with TYPE1 and TYPE2 heatwaves in India (adopted from Ratnam et al. 2016).

Biography

Name: Swadhin Kumar Behera, Application Laboratory/JAMSTEC, Director

Education History: Ph. D. in Oceanography, 1998 / 1988-1997, Researcher at IITM, India and 1998-present in various positions in JAMSTEC.

Academic Highlights/ Major Achievements/ Awards:

Published over 100 scientific articles in reputed international journals with an average citation of 45 and h-index of 33 in web of science. Several awards from JAMSTEC and AGU.

Present Research Interests:

Coupled ocean-atmosphere variability in tropical oceans, variations of ENSO, ENSO Modoki and Indian Ocean Dipole, coastal Nino, air-sea interactions in the subtropical oceans of Southern Hemisphere, tropical and extratropical interactions, climate predictions, climate derivatives and societal application studies.

Contact E-mail: behera@jamstec.go.jp

Potential of Value Generating Toilet Systems

Mahesh Ganesapillai[1], Aruna Singh[1]

[1] Associate Professor, Department of Chemical Engineering, School of Civil and Chemical Engineering, VIT University, Vellore- 632 014, Tamilnadu, INDIA.

email.drmaheshgpillai@gmail.com

The international agenda has neglected the aspects of sanitation and health in its push for (sustainable) development; it isn't surprising to note that 36% of the global population still lacks *access* to improved sanitation facilities. The design and operation of the present day conventional Waste Water Treatment Plants is grounded in philosophy that considers human excreta as 'wastes' and requires treatment, removal from the built environment. The primary objectives of these systems are to (i) ensure minimal exposure of humans to wastes by creating an effective barrier (toilets) and (ii) facilitate appropriate disposal of these wastes through end–of–pipe technologies.

Ecological Sanitation (EcoSan), a concept formulated through an approach that integrates various schools of thought such as circular economy, general systems theory, industrial ecology, biomimicry and life–cycle thinking claims to address the aforementioned shortcomings and initiate a paradigm shift in a way to perceive and manage wastes. Consequently, EcoSan demonstrates a closed–loop methodology for reintroducing resources from wastewater into agriculture rather than letting waste water diffuse into fresh water systems. Although, EcoSan considers technologies as end–points in closing the loop of sanitation, it does not favour any prospects of technological solutions.

Considering the variations in food intake, dietary preferences, geography, demography and socio–economic circumstances, an average human flushes away 4.5 kg of nitrogen (N), 0.5 kg of phosphorous (P), and 1.2 kg of potassium (K) in their toilets. Assuming that an urban setting in a developing country is made up of 20 million inhabitants, if nutrients from these wastes are recovered and recycled, the annual resource savings would amount to 90,000 tons of N, 10,000 tons of P and 24,000 tons of K.

Admitting to the need of an appropriate technological solution(s) that satisfies the aforementioned requirements is vital to achieving circularity in sanitation. To this effect, recent research efforts have been devoted towards the development of technologies that can safely harness nutrients from human excreta to yield usable end products. Consequently, resource–oriented sanitation, or sustainable sanitation, has been advocated as an approach to promote circularity in the flow of (waste) resources from the built to the natural environment. The purpose of this system would be to recycle value–added, nutrient–rich product streams in quantities that ease their management and utilization, in forms that make them plant–available upon application while being free from pathogens and micro–pollutants. Given that the paradigmatic shift in sanitation is reliant upon the development of such solutions, the aim here is to demonstrate a process that makes urine recycling more attractive than the use of synthetic fertilizers in agriculture.

References
[1] O.Cumming, *Desalination*, 2009, 248(1), 8-13.
[2] G.Langergraber, E.Muellegger, *Environment International*, 2005, 31(3), 433-444.
[3] S.A.Esrey, *Water Science & Technology*, 2001,43(4), 177-187.
[4] M.Ganesapillai, P.Simha, A.Zabaniotou, *Sustainable Production and Consumption,* 2015, 4, 36-46.

Biography

Mahesh Ganesapillai is an Associate Professor in the Department of Chemical Engineering at VIT University, Vellore, India, where he has been since 2012 with more than a decade of teaching experience. He received M.Engg. from Annamalai University, Chidambaram in 2002, and his Ph.D. in Chemical Engineering from Anna University, Chennai, India. Later in 2014, he was granted the esteemed Erasmus Fellowship for his Post Doctoral research in Chemical Engineering at the Aristotle University of Thessaloniki, Greece. His research interests center on the closed-loop fertility cycle for sustainability in sanitation and agricultural production through the design and implementation of nutrient recovery systems for the anthropogenic solution. In addition he has made numerous contributions on microwave pretreatment and irradiation; and he has examined the impact of microwave on agricultural biomass, ceramics, food, minerals, medicinal leaves, etc. He regularly acts as reviewer for national and international journals. Prof. Ganesapillai is the author of over thirty four manuscripts on waste management systems. He was awarded the Outstanding Young Chemical Engineer from Indian Institute of Chemical Engineers, the prestigious Senior Research Fellowship award from Defense R&D Organization, Government of India. In 2012 he received the Best Mineral Engineer Award for the development of an outstanding strategy and concept for sustainable agricultural productivity using low grade rock phosphate tailing. Professor Ganesapillai is also a Fellow of the American Institute of Chemical Engineers, Indian Institute of Chemical Engineers, Indian Society for Technical Education, All India Council for Technical Education and the Indian Mineral Engineering Association.

Integrated systems to treat Municipal solid waste (MSW) - An Indian Scenario

Aruna Singh[1], Mahesh Ganesapillai[1]

[1] Associate Professor, Department of Chemical Engineering, School of Civil and Chemical Engineering, VIT University, Vellore -632014, INDIA

email.arunasingh@vit.ac.in

ABSTRACT

Municipal solid waste (MSW) management is one of the foremost environmental problems faced by Indian cities that cause hazards to inhabitants. About 90% of MSW is disposed of unscientifically in open dumps and landfills, creating problems to public health and the environment. The quantity of MSW generated depends on a number of factors such as food habits, standard of living, degree of commercial activities and seasons. In developed countries, very few models considered social aspects of Solid Waste Management focusing solely on the economic and environmental spheres. Involvement of all relevant stakeholders from government, industry and formal private sector service providers to local communities and rag pickers were not considered. It is in this context, a complete waste management cycle from prevention to final disposal is given due consideration. While the need is for 'integrated' methodologies, there is a lack of literature exploring the actual application of post-normal approaches and complex, adaptive systems in developing country contexts. This kind of publicly engaged systems thinking can provide some understanding and create approaches for coping with complexity, while it is not feasible for a cure-all 'solution'.

It is counter-productive for developing countries to use strategies and policies developed for high-income countries. The approaches should be locally sensitive, critical and 'owned' by the community of concern. It is aimed to generate the core evidence on the capability of the complex industrial symbiosis plant to fully recover resources from India's MSW, build around advanced biotechnology processing, accepting a variety of MSW biochemical compositions. Different enzymatic biotechnological solution packages will be available for diverse waste compositions that should be generated by manual at source separating or mechanical processing separation within defined variability limits. The current focus is on the techno-economic assessment of the technology for scalable and feasible outcome.

References

[1] M. Sharholy, K. Ahmad, G. Mahmood, R.C. Trivedi, Waste Management 2008, 28, 459.

[2] A.J. Morrissey, J. Browne, Waste Management, 2004, 24 (3), 297.
[3] J.K. Seadon, Journal of Cleaner Production, 2010, 18 (16–17), 1639.
[4] UN-HABITAT, In: Earthscan (Series Ed.), 2010

Biography

Dr. Aruna Singh is working as Associate Professor in the Department of Chemical Engineering, VIT University, INDIA. After completing her B.Tech in Chemical Engineering from Anna University in the year 1985 she was working as process engineer briefly before doing M.Tech in Food and subsequently PhD in LIT, RTM Nagpur University, India. She has more than 13 years of teaching. She was the Principal Investigator for a project under Women Scientist Scheme-A, Govt. of India that was awarded to women. She has about 12 publications in peer reviewed journals (International). He was guest speaker at many reputed institutes in India, and is a consultant to industrial involved in food processing, waste minimization and management. She has visited more than nine countries to present her research and delivered invited. She is also a visiting professor in Caladonian college of Engineering, Muscat, Sultanate of Oman. Her research interest include food processing, microwave pre-treatment and solar cabinet design and drying. She is also involved in biotechnological intervention to treat waste.

Professor Aruna is also a Fellow of the American Institute of Chemical Engineers (AIChE), Indian Institute of Chemical Engineers (IIChE) and Indian Science Congress (ISC).

Fouling Phenomena in Membrane Filtration and Design of Filters

Kazuho Nakamura

Department of Chemical Engineering, Yokohama National University, Hodogayaku Tokiwadai 79-5, 240-8501 Yokohama , Japan

email.naka1@ynu.ac.jp

In the application of membrane filtration technology to water treatment processes the most important issue is membrane fouling[1]. The membrane fouling can be considered as a surface phenomenon caused by foulants accumulated at membrane surface or pore structure. The phenomena show very complex behaviour because it will depend on type of faulnat, pore size and operating condition[2]. We have studied about properties of the surface phenomena during membrane fouling processes from non-woven fibrous filter to RO membrane in some lab scale experiments[3]. In non-woven fibrous filter the filtration properties were elucidated by the shift of filtration mechanism from depth filtration to cake filtration. In MF membranes the fouling properties depended on type of foulant and showed quite complex behaviour especially for biofouling. In UF membranes the rejected foulants formed gel-layer which will control the filtration properties. In RO membrane the scale was growing at membrane surface and the separation performances of RO membrane were controlled by surface coverage of scale. These observations showed that key points of the fouling phenomena were the place where foulants are accumulated and the behaviour of the accumulated layer of foulants

References

[1] Kazuho Nakamura, Takako Orime, Kanji Matsumoto, Zeta potential monitoring during microfiltration of humic acid, *Journal of Chemical Engineering, Japan,* 45(8), 583-589 (2012).

[2] Kazuho Nakamura, Kanji Matsumoto, Separation Properties of Wastewater Containing O/W Emulsion Using Ceramic Microfiltration/Ultrafiltration (MF/UF) *Membranes,* 3, 87-97 (2013)

[3] Kazuho Nakamura, *Technoscape, Vellore India, October* 20-21 (2016).

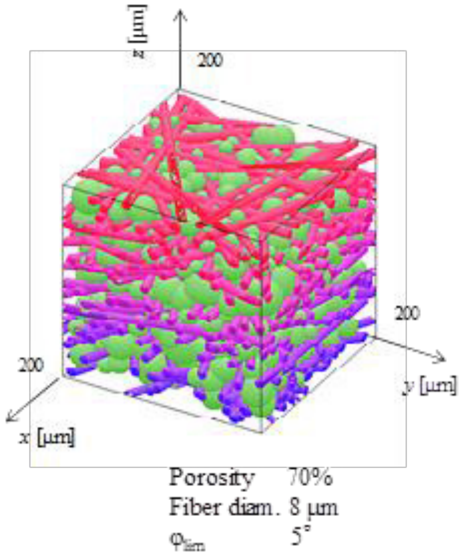


Fig.1 A model for characterization and designing of filter structure in non-woven fibrous filter

Biography

Kazuho Nakamura,
Yokohama National University, Associate Professor

Education History/ Professional History

Bachelor of Engineering (Yokohama National University, 1993), Master of Engineering (Yokohama National University, 1995), Doctor of Engineering (Yokohama National University, 1998)

Application Specialist (Nihon Millipore, 1998-2000), Assistant Professor (Yokohama National University, 2000-2007), Associate Professor (Yokohama National University, 2007-present)

Academic Highlights/ Major Achievements/ Awards

JPI Award for distinguished papers (2012), FTTP (2017)

Present Research Interests

Contact E-mail: naka1@ynu.ac.jp

Adsorbed Natural Gas for Onboard Storage: Tailoring Materials, Challenges and Perspective

K. G. Ayappa
Department of Chemical Engineering, Indian Institute of Science, Bangalore INDIA
email:ayappa@iisc.ac.in

Development of natural gas storage solutions for the transportation sector are important in mitigating global greenhouse gas emissions. The challenge lies in the synthesis of novel nanostructures to meet target gas storage capacities[1]. In order to meet the target capacity requirements and develop a viable technology based on natural gas several challenges have to be overcome. In this talk I will highlight the developments and challenges in this area and give an overview of the multiscale; molecules to transportation approach used in our laboratory. Recent studies have shown that selective functionalization of mesoporous materials such as activated carbons and metal organic frameworks, offers a flexible means to improve their existing gas storage potentials. At the molecular scale, we study gas-solid interactions using ab initio quantum chemical methods and use classical Monte Carlo simulations to obtain gas adsorption isotherms for different graphene based functionalized structures [2]. Our study indicates that specific functionalization can be used to tailor selectivity for gas adsorption and provide a rationale for novel materials design to achieve target storage requirements. In order to evaluate a materials storage capacity, non-equilibrium effects during filling and discharging of onboard canisters must be evaluated and overcome [3]. Adsorption isotherms obtained from the molecular scale are used as input into continuum transport models to understand the heat and mass transfer effects to assess the performance of an on-board adsorbent charge and discharge characteristics.

References

[1] B. P. Prajwal and K. G. Ayappa, ***Adsorption*, 20,** 769–776 (2014).

[2] Debosruti Dutta, Brandon C. Wood, Shreyas Y. Bhide, K. G. Ayappa and Shobhana Narasimhan, ***Journal of Physical Chemistry C***, **118**, 7741-7750 (2014).

[3] P. K. Sahoo, B. P. Prajwal, Siva Kalyan Dasetty, M. John , B. L. Newalkar, N. V. Choudary and K. G. Ayappa, ***Applied Energy***, **15**,190–203 (2014).

Acknowledgements:

This work was supported in part by Bharath Petroleum Corporation Ltd and Department of Science and Technology India.

.

Biography

Name: Ganapathy Ayappa, Professor and Chair, Department of Chemical Engineering, Indian Institute of Science Bangalore India,

Professor Ayappa obtained his Bachelors degree in Mangalore University India and an MS and PhD in Chemical Engineering with a Minor in Mathematics from the Department of Chemical Engineering and Materials Science at the University of Minnesota, in 1992. He was a post-doctoral fellow at the Minnesota Supercomputer Institute and subsequently joined the Department of Chemical Engineering at the Indian Institute of Science in 1993. Professor Ayappa has held visiting positions at the University of North Carolina, the James Franck Institute at the University of Chicago and Department of Materials at ETH Zurich. He is a fellow of the Indian National Academy of Engineers and is currently the Chairman of the Department of Chemical Engineering and Associate faculty in the Center for Biosystems Science and Engineering at the Indian Institute of Science, Bangalore. His research interests lie in developing a molecular understanding of the structure and dynamics of soft matter systems and interfaces using molecular simulations, statistical mechanics and continuum transport models. His research contributions have led to a deeper understanding of materials development for gas storage and separations, carbon capture, structure and dynamics of fluids in nanopores. Recent research efforts involve the use of hierarchical models with a combination of super-resolution spectroscopic methods to study the interactions of proteins with phospholipid bilayer membranes.

Contact email: ayappa@iisc.ac.in

Microscopic Sintering Forces behind Macroscopic Continuum Theory of Sintering

F. Wakai[1], G. Okuma[1], S. Tanaka[2]

[1] Laboratory for Materials and Structures, Institute of Innovative Research, Tokyo Institute of Technology

2Department of Materials Science and Technology, Nagaoka University of Technology

wakai.f.aa@m.titech.ac.jp

Sintering is a thermal process that transforms powder compacts into complex-shaped components. Dimensional control of components is fundamental to meet required tolerance, then, it is necessary to predict dimensions of complex shaped components in order to minimize the grinding/polishing process, so that the machining cost can be reduced. Sintering is described as a deformation at elevated temperatures. In the macroscopic description of deformation, the strain rate is a linear response to applied stress and a thermodynamic driving force, i.e., sintering stress. The continuum theory of sintering is of considerable help in predicting the dimension and shape of products or in designing industrial processes. The sintering stress is a physical quantity that can be determined experimentally by sinter forging tests. It is revealed that the sintering stress and bulk viscosity depend not only on relative density, but also on powder processing.

It is desirable to know sintering stress and viscosity for specific local structure of particle packing. In the initial stage, sintering is described by two-sphere model, where neck is formed, and the neck radius grows with time. The sintering force is the driving force for both shrinkage and neck growth for sintering of crystalline particles by grain boundary diffusion [1], and viscous sintering of glass particles [2]. In the intermediate stage of sintering, the sintering stress can be determined from pore structures in equilibrium states where the mechanical force just balances the surface tension forces so that the porous materials do not shrink. The sintering stress, which is either isotropic [3] or anisotropic [4] can be determined rigorously from the analysis of periodic porous structures. The anisotropic viscosity tensor was also derived from the details of microstructure [5]. However, real porous structures are non-equilibrium, non-periodic, and non-uniform, then, it is still a challenge to estimate sintering stress from the knowledge of microstructures.

Recent advances in X-ray microtomography revealed that the three-dimensional (3D) microstructural evolution during sintering is far more complicated than simplified models. The direct measurement of a 3D structure, which is now readily available from X-ray microtomography, provides a basis for the statistical analysis of microstructural characteristics. The authors have presented methods to estimate sintering stress, either isotropic [6] or anisotropic [7], from the knowledge of microstructure observed by X-ray microtomography base on the theoretical analysis of viscous sintering [8]. We have also found that the topological evolution is described by Euler characteristics as a function of relative density [9]. It provides criteria to distinguish the stages of sintering.

References

[1] F. Wakai, K.A. Brakke, *Acta Mater.,* 59 (2011) 5379.
[2] F. Wakai, K. Katsura, S. Kanchika, Y. Shinoda, T. Akatsu, K. Shinagawa, *Acta Mater.,* 109 (2016) 292.
[3] F. Wakai, Y. Shinoda, T. Akatsu, *Acta Mater.,* 52 (2004) 5621.
[4] F. Wakai, Y. Shinoda, *Acta Mater.,* 57 (2009) 3955.
[5] F. Wakai, T. Akatsu, *Acta Mater.,* 58 (2010) 1921.
[6] G. Okuma, D. Kadowaki, T. Hondo, A. Sato, S. Tanaka, F. Wakai, *J. Am. Ceram. Soc.,* 100 (2017) 867.
[7] F. Wakai, O. Guillon, *Acta Mater.,* 66 (2014) 54.
[8] F. Wakai, *Acta Mater.,* 61 (2013) 239.
[9] G. Okuma, D. Kadowaki, T. Hondo, S. Tanaka, F. Wakai, Sci. Rep., 7 (2017) 11106.

Acknowledgements:

This work was supported by JSPS KAKENHI Grant Number JP26249110.

Biography

Fumihiro WAKAI
Laboratory for Materials and StructuresInstitute of Innovative Research, Tokyo Institute of Technology, Professor

Education History/ Professional History

Kyoto University (BS 1978, MS 1980, Doctor of Engineering 1987)
GIRIN, AIST, MITI 1980-1997
Tokyo Institute of Technology, Professor 1997-present
Director, Laboratory of Materials and Structures 2015-2017

Academic Highlights/ Major Achievements/ Awards

Award Ceram.Soc.Japan (2004), Fellow Am.Ceram.Soc.(2008), World Academy of Ceramics(2012)

Present Research Interests: Sintering, Fracture mechanics, Superplasticity

Contact E-mail: wakai.f.aa@m.titech.ac.jp

Shape Controlled Nanostructures for Electrocatalytic Applications

Raghuram Chetty, Volga Muthukumar, Kranthi Kumar Maniam

Department of Chemical Engineering, Indian Institute of Technology Madras, Chennai, India

Email: raghuc@iitm.ac.in

Polymer electrolyte membrane (PEM) fuel cells have received considerable attention because of their potential application in transportation and portable electronics. The high price and the limited resources of platinum catalysts are among the main challenges that hinder the commercialization of fuel cells. The catalytic properties of nano-materials strongly depend on both the size and shape. The shape plays a more significant role in controlling activity and selectivity, which affect the outcome of the catalysts towards oxidation and reduction reactions in fuel cells. Several conventional wet chemical methods are widely employed for shape controlled nanoparticle synthesis and electrode preparation. These conventional techniques are time consuming, utilize chemicals as reducing agents, and require several post-treatment procedures to remove the unreacted chemicals. In our group, we have employed electrodeposition for electrode preparation, in which catalyst layer is directly formed on carbon coated carbon paper which significantly minimizes the catalyst preparation time and can be directly used as electrodes for fuel cells.

In this talk, an overview of shape controlled nanostructured materials [1] and the recent advances made in our group on controlling the shape of Pt and Pd electrocatalyst on carbon support will be discussed. Pd deposited on an electrochemically functionalized carbon displayed a dendritic morphology with increased electrochemical surface area and showed enhanced catalytic activity for oxygen reduction reaction and formic acid oxidation in comparison to spherical Pd deposit obtained on unfunctionalized carbon [2]. In case of Pt, which was electrodeposited on carbon at three different potentials (viz. 0.2, 0, and −0.2 vs. SHE), the shape of Pt transformed from globular (0.2 V) to dendritic (0 V) and to rosette-like (−0.2 V) structure by increasing the deposition potential in the cathodic direction [3]. Possible reason for the change in shape and the enhanced catalytic activity towards methanol/ formic acid oxidation obtained by the dendritic structure will be presented.

References

[1] S. Nishimura, K. Ebitani, *ChemCatChem,* 2016, 8, 2303.

[2] K.K. Maniam, V. Muthukumar, R. Chetty, *Int. J. Hydrogen Energy,* 2016, 41, 18602.

[3] V. Muthukumar, R. Chetty, *J. Appl. Electrochem*, 2017, 47, 735.

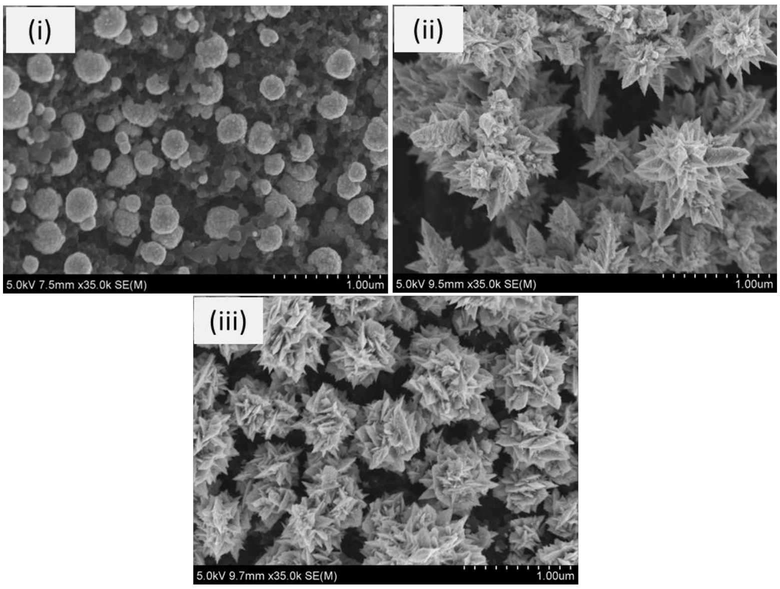


Figure 1. SEM of Pt electrodeposited on carbon black displaying different morphologies namely (i) globular at +0.2 V, (ii) dendritic at 0 V and (iii) rosette at −0.2 V vs. SHE.

Biography

Dr. Raghuram Chetty (Raghu) is an Associate Professor at the Department of Chemical Engineering, Indian Institute of Technology Madras. Raghu has obtained PhD (2004) in Chemical Engineering from Newcastle University, UK and has worked as post-doctoral fellow at Newcastle University, Rühr University Bochum, Germany and Michigan State University, USA. His main research focus is in the areas of electrochemical energy conversion devices especially on fuel cells, exploring on alternative fuels, alternative catalyst and catalyst support (carbon nanotubes, graphene, modified carbon, titania nanotubes), design and assembly of fuel cells. The other areas of interests are in electrochemical and photochemical conversion of carbon dioxide to useful chemicals, hydrogen generation and wastewater treatment. Work from his research group has resulted in 6 patents, 25 research articles and 2 book chapters. Raghu holds professional membership in the ECS, ISE, and RSC.

Machine-learning assisted accurate bandgap predictions of functionalized MXene

Abhishek Kumar Singh

[1]Materials Research Centre, Indian Institute of Science, Bangalore India

abhishek@iisc.ac.in

MXene is a recent addition to the ever-growing family of 2D-materials, and are promising for optical/electronic, energy storage and photocatalytic applications. These early-transition metal carbides and/or nitrides are reactive due to presence of surface charges. Passivation of these by functional groups lends unprecedented functionalities to this class of material simultaneously increasing the number of members in this family by many-fold. Accurate estimate of band gaps is essential to characterize functionalized MXenes for targeted applications. Fundamental band gaps predicted through faster density functional theory (DFT) are usually underestimated. Computationally expensive GW calculations are required to achieve experimental accuracies. Characterizing the electronic properties of MXenes using GW, within a reasonable time, would be practically impossible. Computationally cheaper high-throughput approach could be a powerful tool to filter out the materials in an accelerated and efficient way. Here, we applied machine learning techniques to predict the band gaps of MXenes with GW level of accuracy by utilizing simple and intuitive features. We built a statistical learning model by examining the features with linear/non-linear regressions and identify their important combinations, which predicts the band gaps with minimum root-mean squared error (rmse) within a fraction of time.

References

[1] AC Rajan, A. Mishra, S. S. Gupta, R. Vaish, H. Mizuseki, K-R. Lee, A. K. Singh, to be submitted.

Biography

Name Abhishek Kumar Singh, Materials Research Centre, Indian Institute of Science, Bangalore 560012 INDIA

Education History: / Professional History (career):
06/2016-Present: Associate Professor, IISc, Bangalore, INDIA
06/2010-05/2016: Assistant Professor, IISc, Bangalore, INDIA
06/2010-Present: Adjunct Associate Professor, Materials Science and NanoEngineering, Rice University, Houston, Texas, USA
08/2007–05/2010: Postdoctoral Research Associate, Department of Mechanical Engineering and Materials Science, Rice University, Houston, Texas, USA
03/2006–07/2007: Postdoctoral Research Scholar, Materials Department, University of California Santa Barbara, California, USA
10/2004 – 02/2006: JSPS Postdoctoral Fellow, Institute for Materials Research, Tohoku University, Sendai, Japan
PhD (Computational Materials Science) Institute for Materials Research, Tohoku University, Sendai, Japan 09/2004
MSc (Physics) Indian Institute of Technology Delhi, New Delhi, India 05/2001

Academic Highlights/ Major Achievements/ Awards
06/2015-Present: Editorial board member, Scientific Reports, Nature Publication Group
Materials Research Society of India Medal,2014
JSPS Postdoctoral Research Fellowship, 2004-2006
Monbukagakashu (MEXT) Graduate Research Fellowship, 2001-2004

Present Research Interests
Prof. Abhishek K. Singh has 18 years of experience in multiscale modeling and simulation of materials, using density functional theory, classical and ab-initio molecular dynamics, grand canonical Monte-Carlo simulations and continuum mechanics. He has been involved in understanding theory of defects, impurities, doping and diffusion in bulk and reduced dimensional systems. He has also been working on thermal transport and accelerated discover of novel materials and functionalities using machine learning. He has been focusing on gaining insights into understanding of the mechanisms involved in storing and harvesting energy in functional materials at different length scales.
Contact E-mail: abhishek@iisc.ac.in

Production of $Li^+@C_{60}$

Kaoru Ohno

Department of Physics, Yokohama National University, Yokohama 240-8501, Japan

ohno@ynu.ac.jp

Recently, Li^+ encapsulated fullerene $Li^+@C_{60}$ has attracted considerable interest in the application to thin-film organic solar cells [1], significant enhancement of the Diels-Alder reaction [2], sensor or switch [3], high ionic conductivity [4], and so on. Historically, in 1996, we performed a first-principles molecular dynamics simulation on a Li encapsulation into C_{60} through a six-membered ring [5] and, right after this publication, an experimental evidence of the encapsulation of Li into C_{60} was reported by Campbell et al. [6,7]. However, the global synthesis of $Li^+@C_{60}$ has only become possible with the plasma shower method since 2010 [3]; its production ratio is 1% when Li hits C_{60} with 30 eV kinetic energy. Quite recently we estimated the ideal production ratio of $Li^+@C_{60}$ as a function of the Li kinetic energy and found that its maximum value is 4% in accordance with the ^{7}Li solid NMR experiment [8].

References

[1] K. Ohkubo, Y. Kawashima, H. Sakai, T. Hasobe, and S. Fukuzumi, "Enhanced photoelectrochemical performance of composite photovoltaic cells of $Li^+@C_{60}$ – sulphonated porphyrin supramolecular nanoclusters", Chem. Commun. **49**, 4474 (2013).

[2] H. Ueno, H. Kawakami, K. Nakagawa, H. Okada, N. Ikuma, S. Aoyagi, K. Kokubo, Y. Matsuo, and T. Oshima, "Kinetic Study of the Diels–Alder Reaction of $Li^+@C_{60}$ with Cyclohexadiene: Greatly Increased Reaction Rate by Encapsulated Li^+", J. Am. Chem. Soc. **136**, 11162 (2014).

[3] S. Aoyagi, E. Nishibori, H. Sawa, K. Sugimoto, M. Takata, Y. Miyata, R. Kitaura, H. Shinohara, H. Okada, T. Sakai, Y. Ono, K. Kawachi, K. Yokoo, S. Ono, K. Omote, Y. Kasama, S. Ishikawa, T. Komuro, and H. Tobita, "A layered ionic crystal of polar $Li@C_{60}$ superatoms", Nat. Chem. **2**, 678 (2010).

[4] H. Ueno, K. Kokubo, Y. Nakamura, K. Ohkubo, N. Ikuma, H. Moriyama, S. Fukuzumi, and T. Oshima, "Ionic conductivity of $[Li^+@C_{60}](PF_6^-)$ in organic solvents and its electrochemical reduction to $Li^+@C_{60}^{-}$", Chem. Commun. **49**, 7376 (2013).

[5] K. Ohno, Y. Maruyama, K. Esfarjani and Y. Kawazoe, N. Sato, R. Hatakeyama, T. Hirata and M. Niwano, "All-electron mixed-basis molecular dynamics simulations for collision between C_{60}^- and alkali-metal ions: A possibility of $Li@C_{60}$", Phys. Rev. Lett. **76**, 3590-3593 (1996).

[6] R. Tellgmann, N. Krawez, S.H. Lin, I.V. Hertel, and E.E.B. Campbell, "Endohedral fullerene production", Nature **382**, 407 (1996); E.E.B. Campbell, R. Tellgmann, N. Krawez, and I.V. Hertel, "Production and LDMS Characterisation of Endohedral Alkali-Fullerene Films", J. Phys. Chem. Solids **58**, 1763 (1997).

[7] K. Ohno, A. Manjanath, Y. Kawazoe, R. Hatakeyama, F. Misaizu, E. Kwon, H. Fukumura, H. Ogasawara, Y. Yamada, C. Zhang, N. Sumi, T. Kamigaki, K. Kawachi, K. Yokoo, S. Ono, and Y. Kasama, "Extensive First-Principles Molecular Dynamics Study on the Li Encapsulation into C_{60} and Its Experimental Confirmation", Nanoscale, accepted for publication.

Acknowledgements:

This study was supported by New Energy and Industrial Technology Development Organization (NEDO); the project name is "Investigation of Technological Development of New Nanocarbon Materials in Collaboration of First-Principles Calculations and Experiments" (No. 16101402-0).

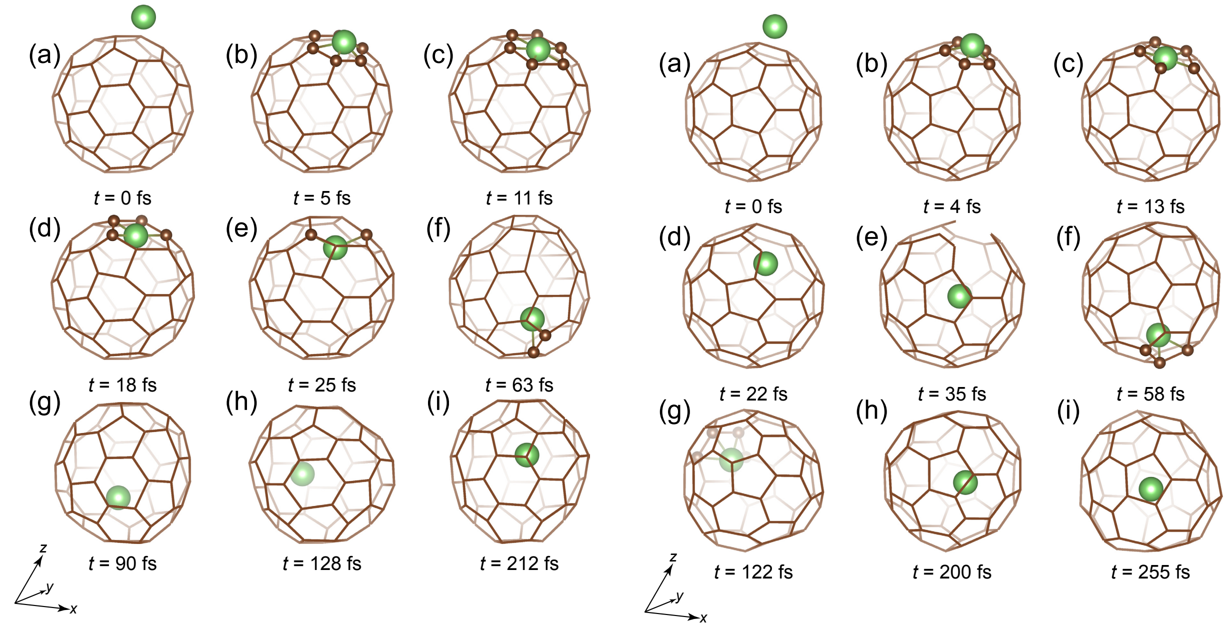


Figure 1. (Left) Snapshots of the simulation, when Li collides at (0.8,0) Å of a six-membered ring at a tilt angle of 36° with respect to the vertical plane of the molecule with an initial kinetic energy of 30 eV. (Right) Snapshots of the simulation, when Li collides at (0.3,0) Å of a five-membered ring at a tilt angle of 21° with respect to the vertical plane of the molecule with an initial kinetic energy of 30 eV

Biography

Kaoru Ohno, Graduate School of Engineering, Professor

(Bachelor Degree) Department of Physics, Faculty of Science, Science University of Tokyo, 1979

(Doctor Degree) Department of Physics, Tohoku University, 1984

(Postdoctoral Researcher) Japan Society of Promotion of Science, 1984

(Assistant Professor) College of General Education, Tohoku University, 1986

(Associate Professor) Institute for Materials Research, Tohoku University, 1990

(Professor) Department of Physics, Yokohama National University, 2000

(Publications) papers 250, books 3 (Kyoritsu/Iwanami in Japanese), 3 (Springer in English)

(Present Research Interests)

(1) Development of an original first-principles code "TOMBO" to calculate optical properties using GW with/without Bethe-Salpeter equation in many-body perturbation theory.
(2) Foreign atom insertion into C_{60}, nanotubes, fullerene polymers and defected graphene.
(3) Potential renormalization theory in cluster expansion of lattice models for alloys and polymers; application to phase field model.

Biocompatible Ferroelectrics as a New Generation Implants for Biomedical Applications

Ashutosh Kumar Dubey[1], B. Basu[2], and K. Kakimoto[3]

[1]Department of Ceramic Engineering, Indian Institute of Technology (BHU), Varanasi-221005, India

[2] Materials Research Center, Indian Institute of Science, Bangalore-560012, India

[3] Department of Materials Science and Engineering, Nagoya Institute of Technology-4668555, Nagoya, Japan

Email: akdubey.cer@iitbhu.ac.in

Owing to the fact that living bone possesses significant electrical activities to govern it's own metabolic processes such as architectural maintenance, growth and fracture healing, the development of bone-mimicking materials attracted significant attention in recent years. Such electro-active materials are expected to ensure the faster and effective post-operative healing process. Towards this end, the present talk will briefly cover the origin of the fundamental electrical responses of living bone as well as the potentiality of multifunctional perovskites such as barium titanate and sodium potassium niobate (NKN) as appealing electroactive alternates in orthopedics. Considering the living cells as an electrical entity, controlled and directed growth and proliferation of cells is speculated to be possible with the externally applied electrical stimulation. The talk will elaborately discuss the number of possible ways to design the electrical equivalent circuits of a living cell based on the path of ions traversed under an applied potential difference. The most important consequence of these analytical studies is that the electric field stimulated cancer treatment as well as enhanced cell proliferation, diametrically opposite effects, can be described.

Further, the talk will elaborate two different aspects of application of electric field in stimulating the growth/proliferation of bone cells as well as connective tissue cells, firstly via intermittent delivery of extremely low strength pulse electrical stimulation and secondly via surface charge generated by electrical poling of ferroelectric-biocomposite substrate. Towards the end, the development of bioactive functionally graded material (FGM) material using a highly ferroelectric ceramic alongwith a comparative assessment of detailed dielectric and electrical behavior will be made in context of the living bone to demonstrate the potentiality of developed FGM as a new generation bioceramic for orthopedic implant applications.

Brief Biography

Dr. Ashutosh Kumar Dubey is currently an Assistant Professor and Ramanujan Fellow in the Department of Ceramic Engineering at Indian Institute of Technology (BHU), Varanasi, UP, India. He earned his PhD from Indian Institute of Technology Kanpur, UP, India in 2012. He was JSPS Fellow at Nagoya Institute of Technology, Nagoya, Japan during 2012-14. He has authored over 30 research papers in peer-reviewed international journals. As recognition of his research work, he received various prestigious awards/fellowships such as Young Scientist Award by Indian Science Congress Association (2011-2012) as well as by Indian Ceramic Society (2015), Japan Society for the Promotion of Sciences (JSPS) Fellowship for Foreign Researchers (2012-14) and Ramanujan Fellowship by Department of Science and Technology, Govt. of India (2015-20).

His research interests includes External electric field and surface charge mediated biocompatibility evaluation of electro-bioceramics, piezoelectric tougheneing of bioceramics, Functionally graded materials, Nanoporous bio-ceramics, Orthopedic biomaterials, Analytical computation.

Contact Details

Dr. Ashutosh Kumar Dubey
Assistant Professor and Ramanujan Fellow
Department of Ceramic Engineering
Indian Institute of Technology (BHU), Varanasi
Varanasi -221005, India
Email: akdubey.cer@iitbhu.ac.in

Surface and subsurface studies of worn SiC based composites for green transport engines systems

B. Venkata Manoj Kumar

Department of Metallurgical and Materials Engineering, Indian Institute of Technology Roorkee, India

E-mail: manojfmt@iitr.ac.in

Owing to the unique combination of light weight, high hardness, high temperature strength and excellent wear resistance, silicon carbide (SiC) ceramics can be used as revolutionary approach for wear-resistant components in fuel injector systems to achieve reduced emissions, improved fuel efficiency and superior engine performance. The wear by incomplete combustion products can be reduced by microstructural engineering. Moreover, the physics of degradation mechanisms is highly dependent on microstructure and mechanical properties of the engineered ceramic system. In the present talk, salient results obtained from tribological behaviour studies of SiC-(0 to 50 wt%) WC composites in continuous sliding wear conditions against strategically selected counterbodies SiC, WC-Co or steel balls will be discussed. Friction and wear results will be explained as function of material composition and sliding test parameters. The subsurface of worn SiC-WC composites will be particularly elucidated to understand dominant wear mechanisms. Against SiC ball, SiC-WC composites showed mechanical fracture as dominant wear mechanism, while worn surfaces of composites revealed tribochemistry with increased WC content against WC-Co or steel ball. Detailed study of sub-surfaces in cross-section modes (using dual-beam focused ion beam (FIB)/FEG-SEM and TEM) underneath surfaces of monolithic SiC and SiC-50wt.%WC composite worn against SiC ball reveals the presence of dislocations and twins in SiC grains in deformation zone beneath the worn region (as induced by the interactive sliding). The WC particles in the composite, in turn, suppress the wear damage by subduing the sub-surface micro-cracking, which otherwise is extensive primarily due to the build-up of stress at the tip of dislocations/twins in SiC grains.

References

[1] S.K. Sharma, B. V. M. Kumar, Y.W.Kim, *Ceram. Inter.* 2015,41,3427.

Acknowledgements:

This work was partially supported by Council of Scientific and Industrial Research (CSIR), New Delhi, India through project No.22(0654)/14/EMR-II.

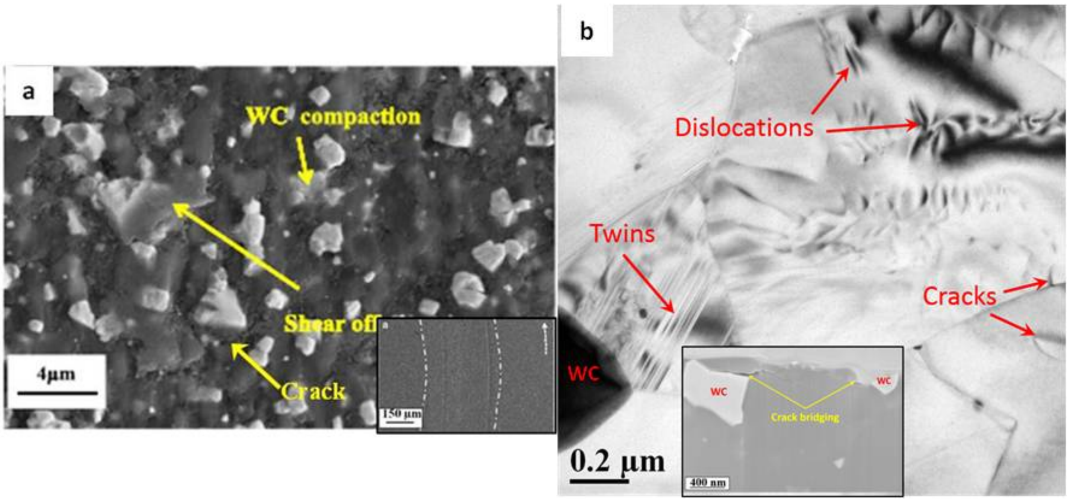


Fig.1. Characteristic features of worn SiC-50 wt% WC composite: (a) cracks in SiC grains and shearing off or compaction of WC particles on surface (b) dislocations, twins and cracks in sub-surface. Inset in (a) shows wear track on worn surface and inset in (b) reveals crack bridging in worn sub-surface.

Biography

Dr. B. Venkata Manoj Kumar is currently working as Associate Professor at Department of Metallurgical and Materials Engineering, Indian Institute of Technology (IIT), Roorkee. Dr. Manoj obtained Ph.D. degree from IIT Kanpur in November 2007. Subsequently, he worked as post-doctoral researcher at Seoul National University from January 2008 to January 2009, Research Assistant Professor at University of Seoul from February 2009 to February 2011, and Assistant Professor at IIT Roorkee from March 2011 to April 2016.

With the primary theme of understanding microstructure-property relations, Dr. Manoj has been actively involved in processing advanced ceramic systems like SiC, ZrB_2, B_4C, Si_3N_4, TiCN-Ni cermets etc., and studying the influence of microstructural characteristics on their material removal mechanisms when subjected to sliding, fretting, erosion or machining conditions. Dr. Manoj has so published more than 50 peer-reviewed research articles in journals of international repute like Journal of the American Ceramic Society, Ceramics International, Science and Technology of Advanced Materials, Acta Materialia etc. He has also presented research work in more than 40 conferences. He is on the panel of reviewers for about a dozen journals of international repute.

Bubble entrapment during liquid drop impact on liquid pool

Hiranya Deka, Gautam Biswas and Amaresh Dalal
Department of Mechanical Engineering, Indian Institute of Technology Guwahati, Guwahati – 781039, India

When a drop of a liquid falls through air to impact on the liquid-air interface of a liquid pool, depending on the size and velocity of the drop, it may become partially or completely coalesced in the liquid, or splash. The transition between complete coalescence and splashing proceeds via a number of intermediate steps, such as thick and thin jet formation and air-bubble entrapment and vortex-ring formation. The impact of the drop on the interface can produce a crater in the liquid pool. The crater produced by the drop impact, expands radially and closes at the top to entrap a large bubble. The large bubble entrapment takes place if the prolate shaped drop impacts onto a liquid pool. Researchers have classified different forms of the bubble entrapment scenario on a velocity versus drop-diameter map (V-D map). On the traditional classification map, the large bubble entrapment zone occupies a small region. Wang et al. [1] experimentally observed large bubble entrapment outside heretofore reported small region of the traditional V-D map. This new finding raised two questions in the mind of the researchers. The first question is, "How does the large bubble entrapment take place?", and second question is, "What is the exact boundary of large bubble entrapment regime on the V-D map?". Thoroval et al. [2] reported that the entrapment of large bubble is a vortex driven phenomena. The vortex deforms the interface and produces an elongated roll jet, which then collapses on the central axis to entrap the large bubble. However, the exact boundary of large bubble entrapment regime on the V-D map is still unexplored. In this work [3] we have attempted to find out the exact regime of large bubble entrapment on the V-D map. Within the given range of aspect ratio variation of the impacting drop, we have been able to draw a conclusion about the boundary of large bubble entrapment regime.

The entrapment of large bubble is always accompanied by a high speed inward jet which is commonly known as Worthington jet and an outward jet. The inward jet and the outward jet start to emerge as the liquid tongue merges at the top of the crater to entrap the bubble. The inward liquid jet moves downward and penetrates the bubble.

References:

[1]. A.-B. Wang, C.-C. Kuan, and P.-H. Tsai, "Do we understand the bubble formation by a single drop impacting upon liquid surface?" Physics of Fluids 25, 101702 (2013)

[2]. M.-J. Thoraval, Y. Li, and S. T. Thoroddsen, "Vortex-ring-induced large bubble entrainment during drop impact," Phys. Rev. E 93, 033128 (2016)

[3]. H. Deka, B. Ray, G. Biswas, A. Dalal, P.-H. Tsai, and A.-B. Wang, The regime of large bubble entrapment during a single drop impact on a liquid pool, Physics of Fluids, Vol. 29, (Issue 9) pp. 092101-1- 092101-13, (2017).

Biography

Prof. Gautam Biswas is currently the Director of IIT Guwahati. He is also a Professor in the Department of Mechanical Engineering at IIT Guwahati and at the Indian Institute of Technology Kanpur. He was the Director of CSIR-Central Mechanical Engineering Research Institute before joining IIT Guwahati. The research group of Professor Biswas at IIT Kanpur identified the phenomenon of Rayleigh-Taylor Instability during the bubble formation in film boiling. This was a significant addition to the classical theory, based on Taylor Helmholtz instability. Professor Biswas is the author of more than 150 technical publications, including more than 100 in the SCI journals. Professor Biswas has completed guidance of eighteen PhD theses and a few are under progress. He is the co-author of an under-graduate level book entitled Introduction to Fluid Mechanics and Fluid Machines (Tata McGraw Hill), and a postgraduate level text book entitled Advanced Engineering Fluid Mechanics (Narosa).

Prof. Biswas was the occupant of the position of GD and VM Mehta Endowed Chair Professor of Mechanical Engineering at the Indian Institute of Technology Kanpur. He was a Humboldt Fellow in Germany in 1987-88 and JSPS invited fellow in Japan 1994. He is a Fellow of the American Society of Mechanical Engineers (**ASME**). He has served a full term as the Associate Editor of the **Journal of Heat Transfer (Trans ASME)**. He was a Guest Professor at the University of Erlangen-Nuremberg in 2002. He was the Dean of Academic Affairs at IIT Kanpur for three years since January 2003.

Prof Gautam Biswas is a Fellow of the all three major science academies of India, such as, the Indian National Science Academy (**INSA**), New Delhi, the Indian Academy of Sciences (**IAS, Bangalore**) and the National Academy of Sciences India (**NASI, Allahabad**). He is a Fellow of the Indian National Academy of Engineering (**INAE**) and Institution of Engineers (**IEI**). He delivered prestigious Prof. **CNR Rao Lectur**e in 2010. He has been awarded the esteemed **J.C. Bose National Fellowship** by the Department of Science and Technology, New Delhi in 2011. He has been awarded the Distinguished Alumnus Award by the Indian Institute of Technology Kharagpur in the year 2016. He has been conferred Honorary Doctorate (**Honoris Causa**) by National Institute of Technology Agartala, India in 2017. Currently he is Associate Editor of a very well-known CFD-journal, - **Computer and Fluids.**

Advanced Materials for Membranes for Cleaner Environment

D.Mohan[1], Noel Jacob Kaleekkal[2]

[1] Hindustan Institute of Technology and Science, Chennai, India, [2] School of Chemical and Biotechnology, SASTRA University, Tanjore, India.

mohantarun@gmail.com, a.deanresearch@hindustanuniv.ac.in

Depleting water resources and an ever increasing requirement have forced us to realize the paramount importance of water treatment. According to the World Bank estimation, nearly 1.1 billion individuals lack access to safe water, which results in millions of diseases or deaths annually by waste water contaminants especially in developing countries [1]. The main environmental contaminants include *metal ions* from chemical, electroplating, refining industries; *oil emulsions* from produced water, oil spills, car servicing centers etc.; *dyes*, *chemical solvents* from textile/manufacturing industries and *proteins and biologically active substances* from pharmaceutical industries. Asymmetric polymeric membranes prepared by phase inversion technique produce membranes of varying pore sizes and properties which can tuned for separation of required contaminant.

Polyamide-imide/TiO_2 [2] Nanofiltration membranes which had exceptional stability to chlorine attack was fabricated for surfactant enhanced removal of divalent salts. Ag nanoparticles [3] were incorporated into PES membranes to prepare NF membranes with enhanced bacterial resistance. Ultrafiltration membranes were employed to break the oil-in-water micro-emulsion and selectively retain oil by employing hydrophilic nano-materials like MWCNTs or amphiphilic polymer Pluronic F127[4] with $CaCO_3$ as a membrane modifier. The resultant membranes showed enhanced water flux while maintaining the required retention of oil droplets. Poly 6-methyl 2-vinyl pyridinium sulphate (PMVPS) cationic polyelectrolyte was introduced into polysulfone membrane to tailor the pore size to effectively improve water flux and anti-fouling ability.

Carboxylated graphene oxide [5] and TiO_2 were assimilated to prepare PEI ultrafiltration membranes and polysulfone Nanofiltration membranes respectively for efficient removal of humic acid. Attempts have been made to correlate the changes in the performance of the membranes with its structure. It is worth mentioning that low free energy membranes prepared by the incorporation of nanoparticles may be valuable for various industrial separations. Epoxidated polyethersulfone (EPES) incorporated cellulose acetate (CA) ultrafiltration membranes were prepared by diffusion induced precipitation technique were demonstrated to be valuable for chromium ion removal [6].

Advanced materials including nano-materials, functionalized long/short chain polymers are effective in tailoring pore sizes of polymeric membranes. They impart mechanical strength, hydrophilicity and increase the fouling resistance of the membrane thereby improving performance and lifetime of the membranes.

References

[1] M.S. Rahaman,, C.D. Vecitis,, M. Elimelech, Environ. Sci. Technol. 46(3) (2012) 1556–64. 10.1021/es203607d.

[2] S. Rajesh,, A. Fauzi Ismail,, D.R. Mohan, RSC Adv. 2(17) (2012) 6854. 10.1039/c2ra20265d.

[3] P. Maheswari,, D. Prasannadevi,, D. Mohan, High Perform. Polym. 25(2) (2013) 174–87. 10.1177/0954008312459865.

[4] J.S.B. Melbiah,, D. Nithya,, D. Mohan, Colloids Surfaces A Physicochem. Eng. Asp. 516(Supplement C) (2017) 147–60. https://doi.org/10.1016/j.colsurfa.2016.12.008.

[5] N.J. Kaleekkal,, A. Thanigaivelan,, D. Rana,, D. Mohan, Mater. Chem. Phys. 186 (2017) 146–58. 10.1016/j.matchemphys.2016.10.040.

[6] A. Jayalakshmi,, S. Rajesh,, S. Senthilkumar,, D. Mohan, Sep. Purif. Technol. 90(Supplement C) (2012) 120–32. https://doi.org/10.1016/j.seppur.2012.02.010.

Biography

Dr. Mohan Doraiswamy Raju
Professor and Associate Dean (Research) HITS & Former Director, Centre for Faculty Development, Anna University, Chennai, India.

Achievements and Awards: **Life-Time achievement Award** -2017 from Institution of Engineers India, **Tamil Nadu Scientist Award**- 2012, **UGC-BSR one time** and **Faculty Fellow** Awards in the years 2012 and 2016, **Active Consultant Award** from Anna University, Chennai in the year 2011 for the valuable contribution to the research and development in Membrane Technology, Japan Society for Promotion of Science (**JSPS**) award April 2004 to Jan 2005. (DST –DAAD) **Senior Scientist exchange program** and visiting Professor at Yokohama National University (2003) Japan.

Present Research Interests: Polymeric membrane development for industrially relevant applications, for bio-medical application

Contact E-mail : mohantarun@gmail.com, a.deanresearch@hindustanuniv.ac.in

Development of titania nanotubes for drug delivery applications

N. Rajendran[1]

1 Department of Chemistry, Anna University, Chennai, India-600 025

rajendranarasi@gmail.com

Drug-releasing implants (DRIs) based on the invention of nanoengineered surfaces on available medical implants have drawn immense interest. Nanotubes and nanoporous structures formed on Al, Ti and their alloys by electrochemical anodization are main platforms for drug releasing implants due to their unique features. Several therapeutic agents such as antibiotics, antifungal, anti-inflammatory, anticancer drugs, bone proteins, peptides, enzymes, vitamins, hormones, genes, antibodies, neurotransmitters, drug nanocarriers and nanoparticles have been applied in order to employ a wide range of therapies into titanium nanotubes based implants. Several reports have described the beneficial effects of quercetin for anti-inflammatory, anti-oxidant, anti-cancer activities and osseointegration property. The biodegradable polymers such as chitosan and PLGA have antibacterial and osseointegration properties. Chitosan's haemostatic properties also allow it to reduce pain by blocking nerve endings. Its properties also allow it to be used in transdermal and controlled drug delivery system. In the present work, Titania nanotubes were loaded with quercetin and covered with biopolymer, chitosan to different thicknesses. Drug release profiles from these samples were studied in Hanks' solution for 192 h. The results showed that drug release into the local environment can be controlled by controlling the thickness of the chitosan and tuned to fit into an optimal therapeutic window for the treatment of post operative infection, inflammation and for quick healing with better osseointegration.

Keywords: chitosan, quercetin, nanotubes drug release.

Reference: L Mohan, C Anandan, N Rajendran, Drug release characteristics of quercetin-loaded TiO_2 nanotubes coated with chitosan, International Journal of Biological Macromolecules Volume 93, 1633-1638 (2016)

Biography

Rajendran Nallaiyan
Professor, Department of Chemistry, Anna University, Chennai
Director, Centre for International Affairs, Anna University, Chennai
PhD in Chemistry, 24 years of academic and administrative experiance

Academic Highlights:

- h-index: 29, Citations: 2600
- Publication: 140
- Conference (National / International): 143
- 23 – PhD Guided

Major Achievements/ Awards:

1. First Awardee - Tushar Jahveri Award – 2017 – NACE East Asia and Pacific Area
2. Meritorious Contribution Award – 2017 – NACE International Gateway India Section, Mumbai
3. Mid-Career Award - 2017 - University Grants Commission – Ministry of Human Resource Development (UGC-MHRD), New Delhi.
4. Tamil Nadu Scientist Award (TANSA) in Chemical Sciences – 2014 -Tamil Nadu State Council For Science and Technology, Chennai, Tamil Nadu
5. Honorary Fellow (2015) – The Academy of Sciences, Chennai
6. MASCOT National Award (2014) – Electrochemical Society of India
7. Meritorious Contribution Award (2014) – National Corrosion Council of India
8. Active Researcher (2013) – Anna University
9. The Excellence in Corrosion Science and Technology (2009 – 2010) – NACE International India Section, Mumbai

Present Research Interests: Biomaterials, Corrosion Science, Electrochemistry and Biomedical Coatings

Email: rajendranarasi@gmail.com / nrajendran@annauniv.edu

Zeolite-Based Nanoporous Materials as High-Performance Catalysts

Yoshihiro Kubota[1], Satoshi Inagaki[1], Naoto Nakazawa[1], Qiao Han[1]

[1] Division of Materials Science and Chemical Engineering, Yokohama National University

e-mail: kubota@ynu.ac.jp

Bulky and rigid quaternary ammonium cations, such as *N,N,N',N'*-tetraethylbicyclo[2.2.2]oct-7-ene-2,3:5,6- dipyrrolidinium (TEBOP^{2+}), as well as less bulky and less rigid cations, such as dimethyldipropylammonium ($Pr_2Me_2N^+$), were used as the organic structure-directing agents (OSDAs) for synthesizing zeolites with Si/Al ratios around 10 or lower. Both TEBOP^{2+} and $Pr_2Me_2N^+$ are effective SDAs for the synthesis of **MSE**-type zeolites, which are applicable as catalysts for selective formation of light olefins, especially propylene, through hexane cracking and dimethyl ether-to-olefin (DTO) reactions [1,2]. It is well-known that the small-pore zeolites with large cavities have found applications in methanol-to-olefin (MTO) or DTO reaction and selective catalytic reduction (SCR) of NO_x. Unlike well-known **CHA**-type zeolites, **AFX**-type zeolites [3,4] with 8-ring channels as well as elongated large-cavity (*aft* cage) and small-cavity (*gme* cage) have not been applied to the DTO and SCR reactions due to the limited Si/Al composition range which arises from a narrow synthesis window. In this work [5], TEBOP^{2+} was firstly used to synthesize **AFX**-type zeolites. As a result, the synthesis window successfully became wider. The product Si/Al molar ratios in the range 6–9 and the dihexahedron-based particle morphology are the remarkable features, which have never been observed in conventional **AFX**-type zeolites. This special **AFX**-type zeolite turned out to be a promising catalytic material for both light-olefin formation and SCR.

The $Pr_2Me_2N^+$ as a simpler OSDA was proven to be effective for production of new zeolite, YNU-5, which is the first zeolite containing interconnected 12-, 12-, and 8-ring pores, as well as independent straight 8-ring channels (Fig. 1) [6]. This material showed promising catalytic performance for dimethyl ether-to-olefin (DTO) reaction.

References

[1] Y. Kubota, S. Inagaki, *Topics in Catalysis*, 2015, 58, 480 and references cited therein.

[2] Q. Han, S. Park, S. Inagaki, Y. Kuobta, J. Petro

[3] R. F. Lobo, S. I. Zones, R. C. Medrud, *Chem. Mater.*, 1996, 8, 2409.

[4] D. W. Fickel, R. F. Lobo, *J. Phys. Chem. C*, 2010, 114, 1633.

[5] N. Nakazawa, S. Inagaki, Y. Kubota, *Adv. Porous Mater.*, 2016, 4, 219.

[6] N. Nakazawa, T. Ikeda, N. Hiyoshi, , Y. Yoshida, H. Qiao, S. Inagaki, Y. Kubota, *J. Am. Chem. Soc.*, 2017, 139, 7989.

Acknowledgements:

This work was financially supported in part by the Japan Science and Technology Agency (JST) for the project of Creation of Innovative Functional Materials with Advanced Properties by Hyper-nano-space Design in the CREST program (project code: JPMJCR1423) and by Grant-in-Aid for Scientific Research (nos. 13199071 and 23760741).

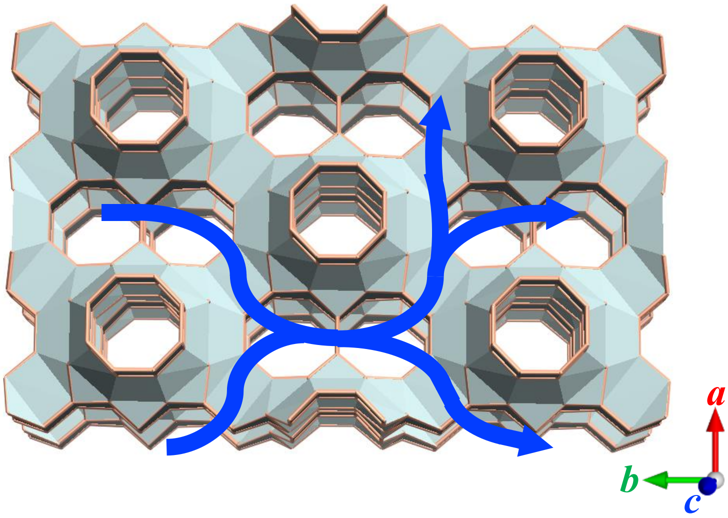


Fig. 1 Schematic illustration of framework and channel architectures of YNU-5 zeolite.

Biography

Yoshihiro Kubota, Yokohama National University, Professor

Education History / Professional History

- Ph.D, University of Tokyo (Pharmaceutical Sciences), March, 1992.
- Researcher, National Institute of Materials and Chemical Research (NIMC), Japan, April 1992 to June 1996.
- Visiting Associate, California Institute of Technology, September 1994-December 1995 (Prof. Mark E. Davis).
- Associate Professor, Department of Chemistry, Gifu University, Japan, July 1996 to August 2004.
- Associate Professor, Division of Materials Science and Chemical Engineering, Yokohama National University, Japan, August 2004 to October 2007.
- Professor, Division of Materials Science and Chemical Engineering, Yokohama National University, Japan, November 2007 to Present.

Awards

- Tokai Chemical Industry Association Award 2001
- The Japan Petroleum Institute, Young Scientist Award 2002
- The Chemical Society of Japan, BCSJ Award 2003

Present Research Interests

Synthesis of ordered microporous and mesoporous materials and their catalytic application---- acid-base catalysis, catalytic oxidation reactions.

Contact E-mail: kubota-yoshihiro-sr@ynu.ac.jp

Surface Modification by Fine Bubble Low Ozonated Water (Fblow®) for Plating on Plastics

Osamu Takai

Materials and Surface Engineering Research Institute, Kanto Gakuin University, Odawara 250-0042, Japan

email. takai@kanto-gakuin.ac.jp

Plating on plastics is widely used in automobile, electronic, decorative and other industries at present. Pretreatment for plastic surfaces conventionally uses chromium acid containing Cr (VI) as surface modification to get strong adhesion between plated layers and plastic surfaces by means of so-called "anchor effect". The chromium acid causes rough surfaces of μm-order that are adequate for the anchor effect.

Recently the chromium acid treatment has, however, two serious problems.

1) Cr (VI) is unusable due to environmental regulations.
2) Smoother modified surfaces on plastics are necessary for electronic circuit boards in preparation for next-generation high speed transmission.

To overcome these problems our research institute has developed new surface modification methods for plastics such as (a) UV or VUV irradiation, (b) radical water treatment and (c) fine bubble low ozonated water (Fblow®) treatment. In this paper we report on the Fblow® treatment for plating on plastics.

The Fblow® treatment uses 1.5-2.0 ppm ozone in fine bubbles for the surface modification of plastics. The low concentration of ozone is sufficient by the combination with fine bubbles. The Fblow® system is shown in Fig. 1. The thickness of modified layers on plastics is nm-order as show in Fig. 2 and by these modified layers the plated layer obtains enough adhesion for industrial applications. After modification ozone decomposes into oxygen and waste liquid treatment is unnecessary. The Fblow®treatment is an environmental-friendly method for the next-generation plating on plastics.

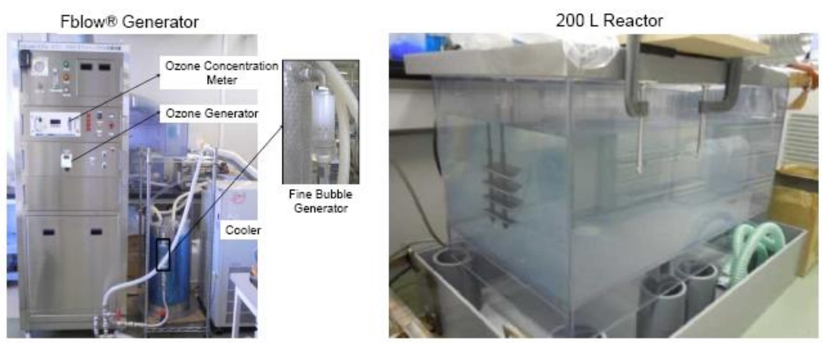


Fig. 1 Fblow® system with a 200 L reactor.

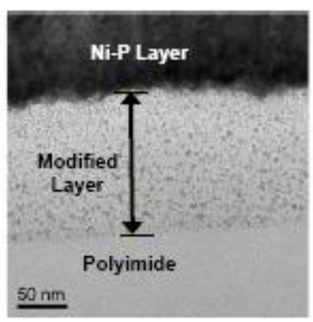


Fig. 2 Cross-sectional TEM image of modified layer for Ni-P plating on polyimide.

Biography

Osamu Takai
Vice Director and Professor, Materials and Surface Engineering Research Institute, Kanto Gakuin University

Education:

1967-1971 Yokohama National University, Bachelor of Engineering
1971-1973 Graduate School, Yokohama National University, Master of Engineering
1973-1976 Graduate School, The University of Tokyo, Doctor of Engineering

Academic carriers:

1976-1987 Research Associate and Assistant Professor, Department of Metallurgy and Materials Science, The University of Tokyo
1987-1992 Assistant Professor and Associate Professor, Department of Mechanical Engineering, Kanto Gakuin University
1992-2004 Professor, Department of Materials Processing Engineering, Graduate School of Engineering, Nagoya University
2004-2010 Professor, EcoTopia Science Institute, and Department of Materials, Physics and Energy Engineering, Graduate School of Engineering, Nagoya University
2010-2012 Director, EcoTopia Science Institute, Nagoya University
2012-to date Vice Director and Professor, Materials and Surface Engineering Research Institute, Kanto Gakuin University

Awards:

Nagai Academic Award, Nagai Science and Technology Foundation (1998)
Plasma Materials Science Award (Academic Award), The 153rd Committee on Plasma Materials Science, Japan Society for the Promotion of Science (2000)
Fellow, The Institute of Physics (2004)
Best Researcher Award, The Surface Finishing Society of Japan (2006)
Achievement Award, National Atomic Energy Committee of Argentina (2007)
President Award, Japan International Cooperation Agency (JICA) (2007)
NISTEP Award (The Researchers with Nice Step), National Institute of Science and Technology Policy (NISTEP) (2010)

Present Research Interests:

Plasma materials processing, Synthesis of advanced materials, Thin film processing, Biomimetic materials processing, Surface Treatment, Water science and technology

Contact E-mail: takai@kanto-gakuin.ac.jp

28-JI-18

Introduction of IIT Guwahati and Collaboration with YNU

Gautam Biswas
Professor, Department of Mechanical Engineering
Director, Indian Institute of Technology Guwahati, India

29-JI-19

International Expansion of Sewage Works in Yokohama

Jungo Kawagoe
Manager, Sewage Works Management Division
Environmental Planning Bureau City of Yokohama

30-JI-20

Water resource conservation and Non-revenue Water reduction

Takeo Tanaka
Manager for International Coordination
Yokohama Waterworks Bureau City of Yokohama

31-JI-21

Nissan Research Activity in India

Fumihiro Haga
Manager, Research Planning Department Research Division
Nissan Motor Co., Ltd.

32-JI-22

FX's New Cellulosic Plastic Technology

Kenji.Yao
Team Manager, New Business Creation
Fuji Xerox

33-JI-23

Role of JICA in Industrial Human Resources Development in India

Takahiro Ikenoue
Senior Deputy Director, Administration Division,
Yokohama International Center,
Japan International Cooperation Agency

Eco-friendly Seed and Crop Fortification Techniques to Augment Biodynamic Farming Systems

Dr.M.Bhaskaran
Vice Chancellor, Tamil Nadu Open University, Chennai-600 015, India

bhaskm@yahoo.co.in / tnouvc@gmail.com

In 1798, Thomas Malthus, predicted that 'arithmetic' increase in food grain production and 'geometric' increase in human population would lead to **chronic food shortages**. Subsequently, in 1880-1900s, **modern plant breeding** methods were developed and public sector also started to invest in crop improvement. This helped to develop continuous stream of high yielding varieties and hybrids. Concomitantly there was an increase in irrigated area due to construction of dams, and increase in usage of chemical fertilizers. All these developments led to substantial increase in food production, thereby avoiding chronic shortage as predicted by Thomas Malthus (1798).

Fall outs of modern agriculture

The hybrid seeds and usage of chemical fertilizers led to much weaker plants which need higher doses of pesticides and fertilizers. Pesticide consumption is low in non-irrigated area. But, in irrigated conditions indiscriminate pesticide spray is adopted especially in commercial crops. Today we are painfully aware of the effects of hybrid varieties and chemical farming. In many places, the soil is getting hard and unable to renew itself so that more and more chemical fertilizers are needed to grow crops, creating huge debts for the farmers. New pests and diseases, resistant to chemical pesticides, are appearing, as are unknown diseases and disorders affecting animals and human beings. We are facing a global disaster, of which many people are becoming aware.

The biodynamic method of agriculture started very slowly but is becoming increasingly popular in the last few decades, all over the world. Biodynamic method was introduced in Germany during 1924 by Dr Rudolf Steiner, Austrian philosopher and scientist. It focuses on substance and energy, well aerated living soil rich in organic matter like humus and cow manure, intelligent crop rotation, cosmic forces, peppering (biodynamical alternative to use chemical sprays) etc.,

Traditional recommendations for implementing Biodynamic farming systems

- Establish environmental control with plant hedges and trees for wind protection, good drainage, water quality, soil-protecting crop rotations, cover crops, compost , green manuring and mulching for weed control.
- Use other preparations such as the Cowpat Pit Preparation, Panchagavya, or natural liquid fertilizers (equisetum tea, fermented nettle manure) as needed.

Recent Eco-friendly Trends

Seeds are the basic inputs of agriculture. Quality seed can directly contribute up to 15-20 per cent to the total crop productivity depending upon the crop. Poor quality seed results in lower seed germination percent and lower seed vigour which ultimately culminates in lower seed yield. It is categorical that seed vigour is the first and foremost factor which decides the productivity potential of the seeds by way of influencing two aspects *viz.,* 1. Seed germination percent and 2) Seedling vigour. Department of Seed Science and Technology of Tamil Nadu Agricultural University in India has developed a series of seed and crop fortification technologies It includes seed enhancement technologies such as i) upgradation of seeds ii) seed priming, iii) seed coating, iv) seed pelleting v) designer seeds and vi) spraying of secondary animal protein extract (Nutrigold) on crop plants. ‘Nutrigold’ product was developed with financial support from Nitta Gelatin India Ltd., Cochin (An Indo-Japanese venture).

References

1. http://agritech.tnau.ac.in/ta/org_farm/orgfarm_biodynmic.html
2. Umarani R. 2010. Seed and crop fortification technologies with KCPL secondary proteins, Project Report, Department of Seed Science and Technology, Tamil Nadu Agricultural University, Coimbatore – 641 003
3. Anon.2017. Seed Enhancement Technologies. Bulletin of Department of Seed Science and Technology, Tamil Nadu Agricultural University, Coimbatore – 641 003

Composite and Functional Silico-aluminophosphate Based Materials: Preparation, Characterization and Its Catalytic Applications

Ayyamperumal Sakthivel,* Maqsood Ahmed, Preeti Sahu

[1] Department of Chemistry, School of Physical Sciences, Riverside Transit Campus,

Central University of Kerala, Kerala 617314, India

email: sakthivelcuk@cukerala.ac.in / sakthiveldu@gmail.com

Aluminophosphate (AlPO) molecular sieves are structurally analogous to zeolites, have better framework flexibility with structural diversity, and are potential catalysts for isomerization, alkylation, and disproportionation reactions.[1] A series of meso-/micro silicoaluminophosphate (Meso-SAPO-*n*) based composite materials and organo-functionalized microporous silicoaluminophosphate (SAPO-*n*-F) materials were prepared from the precursor of microporous silicoaluminophosphate (SAPO-*n*) by hydrothermal method.[2-4] The presence of mesoporosity on Meso-SAPO-*n* material was evident from powder XRD, N_2 sorption and HRTEM analysis.[2] The microporous building unit present on the walls of Meso-SAPO-*n* was confirmed by FT-IR, N_2 sorption studies.[2] The local environment of aluminium and silicon were followed with solid state ^{27}Al, and ^{29}Si MAS NMR spectral studies.[2] The successful incorporation of organo-functionalities on the wall of SAPO-*n*-F framework was confirmed by ^{29}Si and ^{13}C magic angle spinning (MAS) nuclear magnetic resonance (NMR) spectroscopy studies.[3] The developed Meso-SAPO-*n* material shown as potential catalyst for hydroisomerization of 1-octene with about 50% branched isomer selectivity. The kinetic model based on the LHHW mechanism showed that the reaction is first order with respect to 1-octene conversion. Functional SAPO-*n*-F materials found to be effective catalyst for the activation and utilization of CO_2 in cyclic carbonate synthesis from epoxides (98 %) conversion of epichlorohydrin with 96% selectivity toward cyclic carbonate.

References

1. R. Yadav, and A. Sakthivel, Appl. Catal. A: Gen., 481 (2014) 143-160
2. A. K. Singh, K kondamudi, R. Yadav, S. Upadhyayula, A. Sakthivel, J. Phys. Chem. C, 118 , (2014) 27961.
3. R. Yadav, M. Ahmed, A. K. Singh, A. Sakthivel, Scientific Reports, 6 (2016) 22813.
4. M. Ahmed, A. Sakthivel, J. CO_2 Utilization, 22 (2017) 392.

Acknowledgement: Author thank to DST-SERB (EMR/2014/001214) for the financial support.

Biography

Dr. Ayyamperumal Sakthivel

Associate Professor,

Department of Chemistry, School of Physical Sciences

Central University of Kerala, 671314, Kerala

Mobile: 8527103259 /7907682580,

E-mail: sakthiveldu@gmail.com / sakthivelcuk@cukerala.ac.in

URL: http://cukerala.ac.in/images/chm/Chemistry/Dr.Sakthivel_CV.pdf

Education History (educational background)

Ph. D. (Chemistry) from Indian Institute of Technology-Bombay, Mumbai, 2002.

M. Sc. (Chemistry) from Madurai Kamaraj University (Madurai), 73.3 %, 1997

B. Sc. (Chemistry) Madurai Kamaraj University, Madurai, 79.1 %, 1995.

Professional History (career)

Associate Professor : Head (Jan. 2016-April 2017), Department of Chemistry, CENTRAL UNIVERSITY OF KERALA, Kerala 671314, India, **(since 29th January 2016 –present)**

Assistant Professor : DELHI UNIVERSITY, Department of Chemistry, Delhi, Nov.2010–28thJan. 2016.

Senior Manager (R &D) : RELIANCE INDUSTRIES Ltd., India Jun 2008 – 30th October 2010.

JSPS Research Fellow : Department of Chemistry, Gifu University, Japan, Sep-2006 to June 2008.

Alexander von Humboldt Fellow: Department of Chemistry, TUM- Germany, 01-03-2004 to 31-07-2006.

Post-doctoral Research Fellow: IAMS, Academia Sinica, Taipei, Taiwan, Oct. 2002 to Jan. 2004.

Academic Highlights/ Major Achievements/ Awards

- **Mayadevei Juneja Endowment Medal Award – 2017,** **I**ndia Association of **S**olid State **C**hemists and **A**llied **S**cientists (ISCAS), India
- ***Dr. Sistla Kameswari Young Scientist Award – 2015*****,** Catalysis Society of India, **India**
- Published research articles **90** in international peer-reviewed journals
- H-index of **28;** Total citation of **2400**
- Book chapters written **03 ;** Book **01**
- No of external projects **4;** Number of Ph.D./ M.Tech / M.Sc **04 / 02 / 06**

Present Research Interests

- Inorganic Materials (synthesis & characterization of nano-porous & size materials)
- Development of eco-friendly heterogeneous catalysts for fine & petrochemical processes.
- Nano particles synthesis & its catalytic application for hydrogenation / hydroformylatio
- Heterogenization of homogeneous catalysts

Contact E-mail: sakthivelcuk@cukerala.ac.in/ sakthiveldu@gmail.com

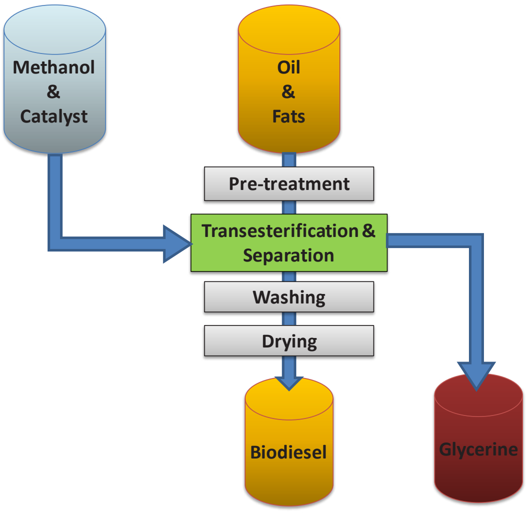
Porous Catalytic Materials for Biodiesel Production

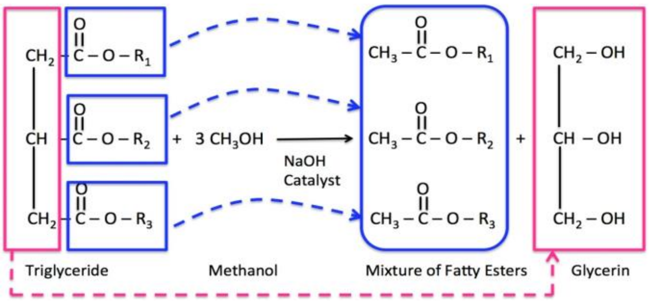
Rajib Bandyopadhyay[1], Sunita Barot
[1] Pandit Deendayal Petroleum University, School of Technology, Gandhinagar, Gujarat, India
Email: rajib.bandyopadhyay@sot.pdpu.ac.in

Synthetic porous materials are widely used as catalysts in the chemical processes of petroleum, pharmaceutical, food and polymer industries etc. Biodiesel, composed of mono alkyl esters of fatty acids derived from vegetable oils /animal fats, has cardinal potential as alternative fuels. The present work explores the synthesis and application of acidic and alkaline functionalized solid catalysts for transesterification reaction and thereby development of efficient heterogeneous catalysts for transesterification of triglycerides. Various porous catalytic materials were synthesized, modified and successfully applied for transesterification of model triglyceride (Triacetin) as well as complex triglycerides (Jatropha oil). Modified materials such as metal (K, Li, Cs) impregnated nano-Silicalite-1 zeolites showed excellent alkaline properties with high reactivity in transesterification reaction of both triacetin and Jatropha oil. The order of catalyst reactivity was found in order of KS >LS >CS. 3 % metal loaded catalyst have given maximum conversion in each case. In solid acid category super acidic sulphated zirconia was synthesized and utilized for transesterification of triacetin. It showed 96 % conversion at, 1:15 triacetin to alcohol molar ratio at 70 °C temperature with 10 wt% catalyst loading in 3 h of reaction time. Mesoporous ordered siliceous material MCM-48 was synthesized in present work and modified with organic surfactants with active alkaline (MCM-48NH2) and acidic (MCM-48SO3H) group. This organic-inorganic hybrid was found to be active catalyst for the transesterification of triacetin. Among the studied and tested catalyst potassium loaded nano-Silicalite-1 was the novel and best catalyst for transesterification of triacetin as well as Jatropha oil. Heterogeneous nature of catalyst was certified by its leaching test. The catalyst is not sensitive to FFA or moisture content of feed stock and reacts at mild process parameters. KS-3 catalyzed process follows first order kinetics and with relatively low activation energy. The catalyst opens a new insight into the field of solid base catalyst with green chemical application in biofuel synthesis.

The present research work directs towards green biofuel technology from sustainable biomass that is eco-friendly in long run. The current studies are helpful for research groups in both work area ‘catalyst development’ as well as ‘biofuel development’.

References
[1] S. Barot, R. Bandyopadhyay, S. S. Joshi, *Environ. Prog. Sustain. Energy*, 2017, 36, 749.
[2] S. Barot, M. Nawab, R. Bandyopadhyay, *J. Porous Mater.*, 2016, 23, 1197.
[3] S. Barot, R. Bandyopadhyay, *Nanoscience and Nanotechnology*, 2016, 6, 110.





Biography

Dr. Rajib Bandyopadhyay, Professor & Head, Department of Science, School of Technology, Pandit Deendayal Petroleum University, Gandhinagar, Gujarat, India
Email: rajib.bandyopadhyay@sot.pdpu.ac.in

Dr. Rajib Bandyopadhyay has been working in the School of Technology, PDPU since 2010. He received his PhD degree from National Chemical Laboratory (NCL), Pune in 1997. Later he did postdoctoral research in Japan (NEDO and JSPS Fellow) for four years followed by Germany (Alexander von Humboldt Fellow). Before joining PDPU, Dr. Bandyopadhyay worked in senior management position in the R&D sectors of various multinational companies including Sud-Chemie, Owens Corning and Sika. He is a life member of International Zeolite Association. His areas of research interest are Heterogeneous catalysis, Materials chemistry, Zeolites and other porous materials, their synthesis and application in fine chemicals, petroleum refining and biofuel synthesis

Role of CO_2 as a Soft Oxidant for Oxidative Dehydrogenation Reaction of Lower Hydrocarbons Over Mixed Metal Oxide Catalysts

Raja Thirumalaiswamy, Ashok kumar V and Aswathy TV

Catalysis and Inorganic Chemistry Division, CSIR-NCL, Dr. Homibhaba road, Pune- 411 008, INDIA

email t.raja@ncl.res.in; traja58@gmail.com

The enormous reserves and the low cost of natural gas raised an increasing interest towards the processing of its hydrocarbon components, namely methane and lower amounts of ethane, propane, butanes.[1] Olefins, being an important starting material in petrochemical and polymeric industry increase the demand in the global market and thus lead to the alternative solutions for the production. Current production of olefins is from the high temperature catalytic cracking of paraffins. As a second source the catalytic dehydrogenation of alkanes suffers from thermodynamic limitation which requires high temperature (>600ºC) and it can result in the formation of more byproducts and immediate catalyst deactivation.

Oxidative dehydrogenation (ODH), an alternative solution to this problem overcomes these limitations mainly because of its exothermic [2] as well as irreversible nature (ΔH^o= -116.7 kJ/mol, ΔG^o= -176.1 kJ/mol). Introduction of an oxidant into the reaction mixture allows the produced hydrogen to oxidize which makes it exothermic and in turn reduces the side reactions. Carbon deposition which is the main reason for catalyst deactivation can be minimized in ODH by the use of various oxidants thereby improving the catalyst stability.

Many efforts have concentrated on the use of CO_2 as an attractive building block for many chemicals. However it can also be used as an oxygen transfer agent or as a soft oxidant.[3, 4] By using CO_2 as a soft oxidant for oxidative dehydrogenation reaction of hydrocarbons, coke deposition can be eliminated and the reduced active phase can be reoxidised. Unlike O_2, it can effectively prevent the deep oxidation of hydrocarbons and improve the stability of catalysts. But the development of a suitable catalyst to activate CO_2 and to maintain the selectivity of olefins produced is highly desirable and a challenge.

References

[1] S.H. Chan, H.M. Wang, *Fuel Process. Technol. 2000*, 64, 221.

[2] O. Ovsitser, E.V. Kondratenko, *Chem. Commun.*, *2010*. 46(27) 4974-4976.

[3] M. B. Ansari, S. E. Park, *Energy Environ. Sci.*, *2012*, 5, 9419-9437.

[4] S. Wang, Z. H. Zhu *Energy Fuels*, *2004*, 18 (4), 1126–1139.

Acknowledgements:

This work was supported by DST, NMITLI - Government of India

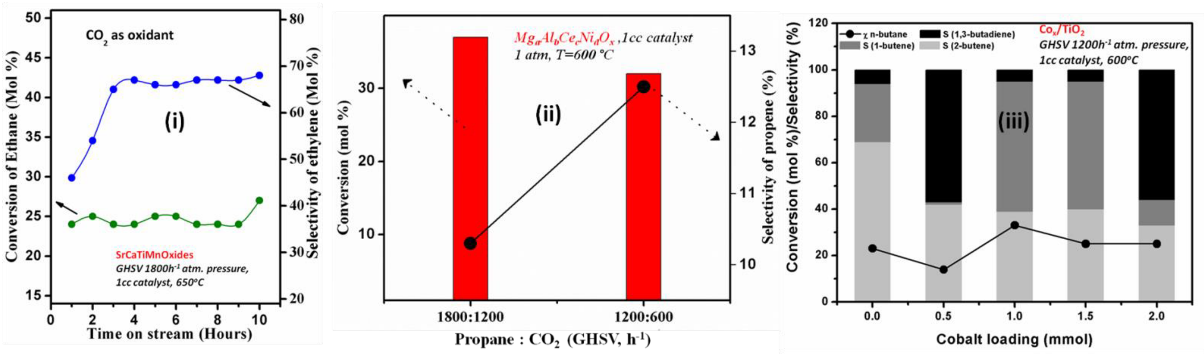


Figure.1. Oxidative dehydrogenation of (i) ethane, (ii) propane and (iii) n-butane using CO_2 as soft oxidant over various mixed metal oxide catalysts

Biography

Raja Thirumalaiswamy, CSIR- NCL, Senior Scientist

Ph.D., Catalysis / JSPS Fellow

Recipient of CSIR Technology award (2015), Government of India

Alternative fuels (Biodiesel, DME) and ODH reactions for lower hydrocarbons, Selective oxidation and reduction reactions

Contact E-mail: t.raaj@ncl.res.in ; traja58@gmail.com

Chemical Design of Layered Double Hydroxide Nanoparticles for Water Purification

Yoshiyuki Kuroda[1]

[1] Green Hydrogen Research Center, Yokohama National University, 79-5 Tokiwadai, Hodogaya-ku, Yokohama 240-8501, Japan.

kuroda-yoshiyuki-ph@ynu.ac.jp

Purification of water from toxic elements is one of the most important issues in the world. Although many kinds of inorganic ion exchangers have been proposed to remove toxic elements from water, most of them are cation exchangers; thus, useful inorganic anion exchangers are highly demanded. Layered double hydroxides (abbreviated as LDHs; e.g., $Mg_{1-x}Al_x(OH)_2 \cdot A^{n-}{}_{x/n} \cdot yH_2O$; A is an exchangeable anion.) are expected to be used for the removal of anionic species (e.g., AsO_4^{3-}, SeO_4^{2-}, $B(OH)_4^-$, and F^-) from water; however, due to the strong affinity of LDHs with CO_3^{2-}, their anion exchangeability is deteriorated under ambient conditions. A previous study has suggested the anion exchangeability of small LDH particles under ambient conditions,[1] though no useful method for precise control of particle size of LDHNPs (LDHNPs) have been reported. Here, I demonstrate a novel method to control particle size of LDHNPs and its effect on the anion exchangeability under ambient conditions.[2,3]

LDHNPs were synthesized by a simple method where an aqueous solution of metal salts ($MgCl_2$ and $AlCl_3$) was mixed with that of a tripodal ligand (tris(hydroxymethyl)-aminomethane; THAM), followed by heating at 80 °C for 24 h. Uniform LDHNPs with precisely controlled sizes were obtained by this method. The average particle size was 10 and 26 nm when the concentration of THAM was adjusted to 0.50 and 0.25 M, respectively (Fig. 1). THAM was immobilized on the outer surface of each LDHNP; thus, it is suggested that THAM efficiently suppresses the crystal growth of LDHNPs, depending on its concentration. A conventional LDH particle whose average size was 107 nm was also prepared.

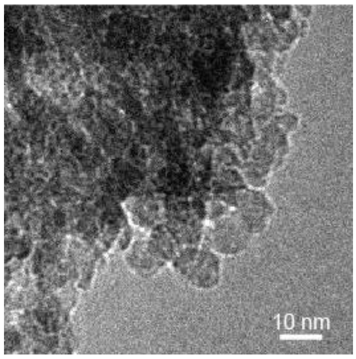


Fig 1. TEM image of the LDHNP ca. 10 nm in size.

To assess the practical anion exchangeabilities of LDHNPs and a conventional LDH, CO_2 was not excluded from the system, no additives (e.g., mineral acids and buffer solutions) were used, and only water was used as a solvent for all the following anion exchanging experiments. The LDHNPs exchanged their interlayer CO_3^{2-} with NO_3^- even though they were exchanged with CO_3^{2-} prior to the experiment (Fig. 2). The conventional LDH could not exchange at all.

Therefore, only LDHNPs could exchange CO_3^{2-} with other anions, which means not only their high performance for anion exchange but also that they can be regenerated by simple anion exchange treatment even if they are deactivated by CO_3^{2-}. The CO_3^{2-} locating at the edge of a particle is thought to be readily exchangeable, and the size reduction can increase the amount of edge sites.

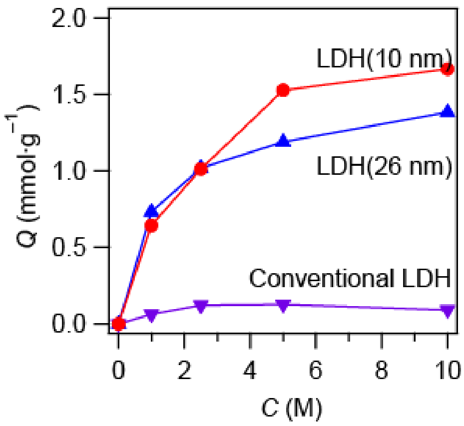


Fig. 2. Exchanged amount of NO_3^- (Q) plotted against the initial concentration of $NaNO_3$ (C).

The removal of harmful anions, such as AsO_4^{3-}, SeO_4^{2-}, and $B(OH)_4^-$, from water was also investigated. The final concentrations of AsO_4^{3-} and SeO_4^{2-} treated by the LDHNPs satisfied the WHO standard for drinking water. Although $B(OH)_4^-$ is known as one of the most difficult anions to be removed from water, the final concentration after double treatment by the LDHNPs satisfied the national effluent standard in Japan. The LDHNPs could be recovered by filtration and reusable at least for 3 times without loss of anion exchangeability.

Consequently, the use of molecular-level interactions between inorganic crystals and organic molecules is key to control the morphologies of LDHNPs. The LDHNPs are found to be useful for purification of water from anionic species under ambient conditions.

References

[1] T. Hongo, M. Takahashi, A. Yamazaki, *Chem. Lett.* 2006, 35, 1296.

[2] Y. Kuroda, Y. Miyamoto, M. Hibino, K. Yamaguchi, N. Mizuno, *Chem. Mater.* 2013, 25, 2291.

[3] Y. Kuroda, K. Yamaguchi, K. Kuroda, N. Mizuno, Bull. Chem. Soc. Jpn. 2015, 88, 1765.

Biography

Yoshiyuki Kuroda, Associate Professor, Green Hydrogen Research Center, Yokohama National University

2011 Ph.D. at Waseda University, 2011–2014 Postdoctoral researcher at the University of Tokyo, 2014–2017 Associate Professor at Waseda Institute for Advanced Study, and from 2017 at the current position.

Interests: Precise synthesis of inorganic nanospace materials.

Award: CerSJ Award for Young Scientists from the Ceramic Society of Japan (2015).

Contact E-mail: kuroda-yoshiyuki-ph@ynu.ac.jp

Selectivities in Adsorptions Induced by Surface Curvature of Functionalized Mesostructured Silica

Hideaki Yoshitake[1]

[1] Division of Materials Science and Chemical Engineering, Yokohama National University

e-mail: yos@ynu.ac.jp

The functionalization of silica surface has been extensively studied for several decades, because it is an excellent combination of a stable high-surface-area solid and chemical specificities of organic functional groups. Ordered mesoporous silica has been also widely used for the functionalization for the same reason. [1-5] However, although the uniform concave surface in the nanometre scale is clearly one of the most prominent characteristics of mesoporous silicas, these characteristics have rarely been emphasized in the applications of mesoporous silica. In order to shed light on the uniform surface coverture, we grafted two 3-aminopropylsilane molecules, after being coupled with a benzenedialdehyde, on mesoporous silicas and, after the removal of benzenedialdehyde by hydrolysis, we carried out the adsorption of the isomers of benzenedialdehyde. Furthermore, we prepared several kinds of N-aminoethyl-3-aminopropyltriethoxysilane-coordinated Fe^{3+} and Cu^{2+} complexes and grafted them on mesoporous silica. These adsorbents were used in the adsorption of for benzenedialdehyde and toxic oxyanions.

We coupled two 3-aminopropylsilane molecules using m- and p-isomers of benzenedialdehyde. A significant heat formation was observed during the coupling reaction at room temperature. These coupled disilanes were analysed by ^{13}C-CP MAS NMR and FT-IR, in addition to CHN elemental analysis. We confirmed the structures of as-grafted and after-extraction solid. The transition metal complexes were formed by mixing at room temperature. The structures were analysed by the same methods with coupled silanes.

In the adsorption of p-benzenedialdehyde, the Langmuir coefficient is larger on 3-aminopropylsilane-grafted SBA15, whose grafts are coupled with p-benzenedialdehyde, than on the equivalent SBA15 prepared using the grafts coupled with m-benzenedialdehyde. This equilibrium constant for m-benzenedialdehyde adsorption is larger on 3-aminopropyl-SBA15 prepared using the disilane with m-benzenedialdehyde than on 3-aminopropyl-SBA15 prepared with p-benzenedialdehyde. Although the conformational changes of NH_2-CH_2-CH_2-CH_2-Si chain provides various orientations of the loan pair on nitrogen, the distinct selectivity change in the adsorption observed on SBA15 substrate implies that the a pair of organic tethers fit to the aldehyde functions of the adsorbate by adjusting their conformations. On the other hand, using Cab-O-sil M7D non-mesoporous silica instead of SBA-15, little change in the Langmuir coefficient was found between the adsorbents. The intensities of IR absorption bands for –C=N-after the adsorptions were stronger (, in comparison with –CH=O stretching modes,) in the adsorption on 3-aminopropyl-SBA15s than on 3-aminopropyl-M7Ds, when the template isomer is the same as the adsorbate molecule. This result suggests that the difference between two silica substrates is attributed to the orientations of 3-aminopropyl functions, which is likely induced by the concave surface of SBA15.

The adsorption capacity of oxyanion is generally stoichiometric on N-aminoethyl-3-aminopropyl-cooridnated transition metal complexes attached on SBA-15. Moreover, the stoichiometry changes according to the coordination number of AeAP functional group. However, these phenomena were not observed the same complexes attached on M7D silica; the adsorption capacity is not stoichiometric and the no significant difference in the adsorption isotherms between the metal complexes with a different coordination number of AeAP group. These adsorption characteristics found only on mesoporous silica substrate are also well explained by the surface curvature.

References

[1] H. Yoshitake, “Highly-controlled synthesis of organic layers on mesoporous silica: their structure and application to toxic ion adsorptions.” *New J. Chem.*, **29**, 1107 – 1117 (2005).

[2] H. Yoshitake, “Nano-Fabrication of Organic Layers on Mesoporous Silicas developed for Adsorption of Environmentally Toxic Oxyanions.” K. Ariga and H. S. Nalwa, ed., *BOTTOM-UP NANOFABRICATION: Supramolecules, Self-Assemblies, and Organic Film.,* vol. 6, Chapter 10, American Scientific Publishers, Stevenson Ranch CA, 2009.(January 2009)

[3] H. Yoshitake, “Functionalization of Periodic Mesoporous Silica and Its Application to the Adsorption of Toxic Anions” G. E. Fryxell and B. Cao ed. *Environmental Applications of Nanomaterials*, *Synthesis, Sorbents and Sensors.* 2 nd Edition, Chapter 11, Imperial College Press, London, 2012.

[4] H. Yoshitake, “Design of functionalization and structural analysis of organically-modified siliceous oxides with periodic structures for the development of sorbents for hazardous substances.” *J. Mater. Chem.* **20** (22), 4537-4550 (2010).

[5] T. Kodate, K. Sato, H. Yoshitake, “Enhanced selectivities in adsorptions of inorganic ions and organic molecules on functionalization of the surfaces of mesoporous silicas.” Advanced Porous Materials, 1(4), 323-336 (2013).

Pre and Post-Symposium Events

December 12 (Tue)

10:30-11:00
Courtesy call

12:00-13:00 Lunch

13:00-16:00
Campus Tour, Laboratory Visiting, Short Lectures for Students, Collaboration Meeting

December 15 (Fri)

Japan-India YNU Symposium 2017

GMI Symposium 2017

8:00-20:00
Company Tour to NTC (Nissan Technical Center)
http://www.nissan-global.com/EN/index.html

Excursion to Hakone, View of Mt. Fuji
http://www.pixpot.net/articles/u_d_view/133/taikanzan

Visit to Materials & Surface Engineering Research Institute, Kanto Gakuin University
http://mscenter.kanto-gakuin.ac.jp/

December 15 (Fri)

YEIS International Forum 2017

Venue: "**YNU Minato-Mirai Campus ", Yokohama Landmark Tower**

Chair: Chair: N. Tamura

9:00 34-YEIS-11 Observing cyber attacks in IoT
Katsunari Yoshioka
Yokohama National University, Japan

9:20 35-YEIS-12 ECOLOG: A database of EV energy consumption log acquired by vehicle mounted sensors
Takashi Tomii
Yokohama National University, Japan

9:40 **Discussion**

Participants from India

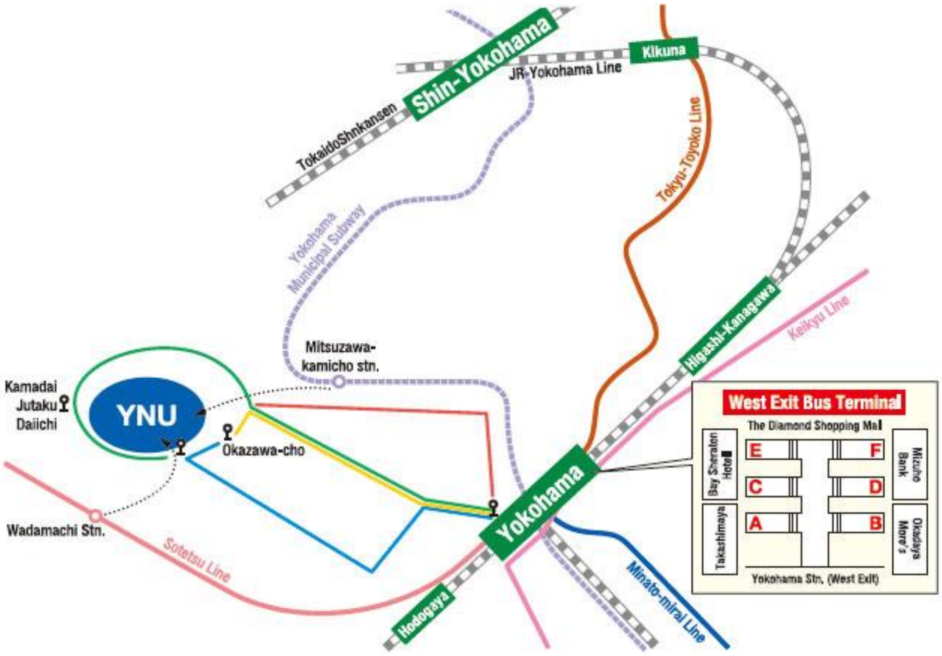
State	Affiliation	Name
CBIC Tamil Nadu Karnataka	IIT Madras	Prof. A. Kannan
	IIT Madras	Assoc. Prof. Raghuram Chetty
	Anna U	Prof. N. Rajendran
	Hindustan U	Prof. D. Mohan
	Tamil Nadu Open U	Vice Chencellor, Dr.M. Bhaskaran
	VIT U	Assoc. Prof. Mahesh Ganesapillai
	VIT U	Assoc. Prof. Aruna Singh
	IISc	Prof. K Ganapathy Ayappa
	IISc	Assoc. Prof. Abhishek Singh
Assam	IIT Guwahati	Director, Prof. Gautam Biswas
Gujarat	PDPU	Prof. Rajib Bandyopadhyay
Kerala	Central U Kerala	Asscoc. Prof. Ayyamperumal Sakthivel
Maharashtra	NCL	Dr. Thirumalaiswamy Raja
Uttarakhand	IIT Roorkee	Assoc. Prof. B. Venkata Manoj Kumar
Uttar Pradesh	IIT Varanasi	Assoc. Prof. Dubey Ashutosh Kumar

http://www.fssai.gov.in/

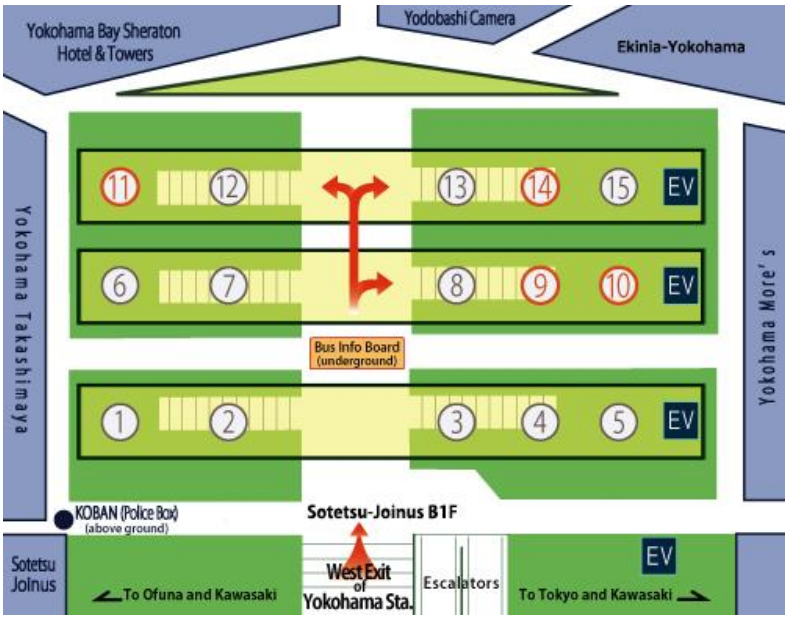
Campus information, Map, Access

How to reach YNU from Yokohama Station

By Train
To the Main Entrance
The Nearest Station:
[Yokohama Municipal Subway]
Mitsuzawa-kamicho Station
About a 16 min. walk

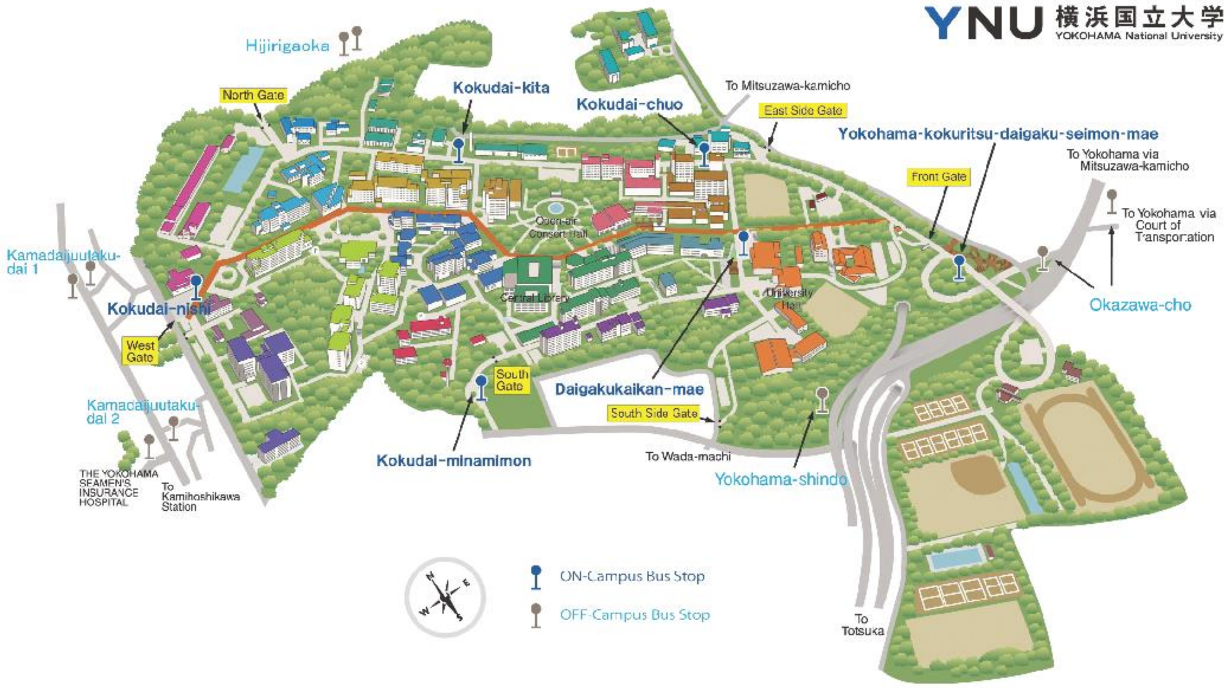


By Bus / Taxi
(The West Exit of Yokohama Station) .
It takes 15-20 minutes from the bus terminal at the West Exit of Yokohama Station to YNU



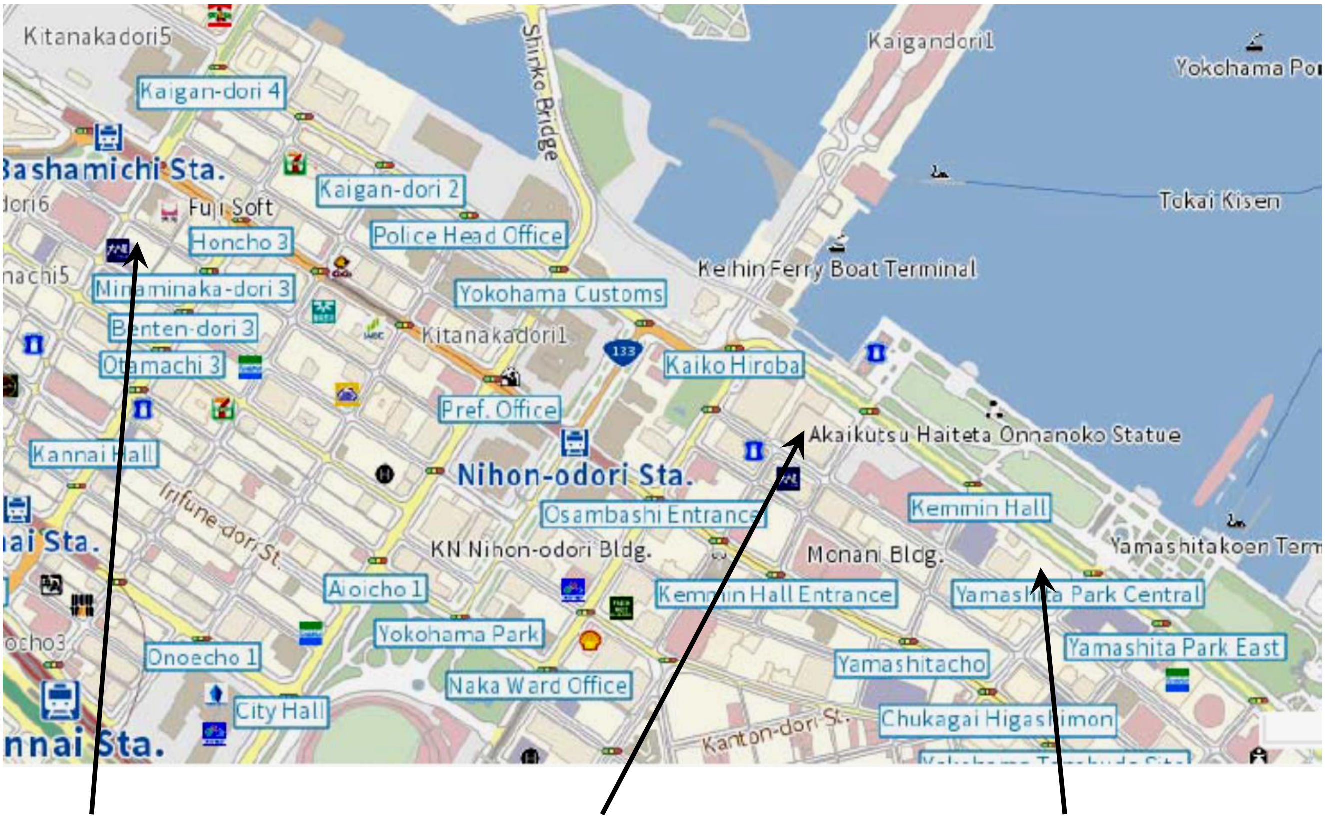
http://www.ynu.ac.jp/english/access/index.html

Campus Map



http://www.ynu.ac.jp/english/access/map_campus.html

Hotels and Venue of the Symposium



Hotel Route-Inn Yokohama Bashamichi

Yokohama Symposia (Symposium venue)

Hotel New Grand

JICA Yokohama

Address: 3-1, Shinko 2-chome, Naka-ku, Yokohama 231-0001

MAP from Yokohama Symposia to JICA Yokohama

Organizing Committee

Advisory:

Prof. Fuminiko Nakamura, Vice President &
Intern. Strategy Org. Executive Director, YNU
Prof. Seiya Negami, Dean, Env. & Info. Sci. (EnvInfoSci) , YNU
Prof. Masayoshi Watanabe, Dean, Eng. , YNU
Ms. Tomoko Takeuchi, Manager, International Office, YNU
Prof. A. Kannan, IIT-Madras
Prof. N. Rajendran, Anna Univ.
Prof. Bikramjit Basu, IISc

Organizing Committee at YNU:

Prof. Meguru Kaminoyama, Eng. Chairperson
Prof. Atsushi Suzuki, EnvInfoSci Co-chairperson
Prof. Hideaki Yoshitake, Eng. Secretary in General
Prof. Junichi Tatami, EnvInfoSci Program
Prof. Yoshihiro Kubota, Eng. Program
Assoc. Prof. Kazuho Nakamura, Eng. Treasurer
Prof. Koichi Nishino, Eng.
Prof. Kaoru Ohno, Eng.
Assoc. Prof. Kenji Aramaki, EnvInfoSci
Assoc. Prof. Motoyuki Iijima, EnvInfoSci
Assoc. Prof. Akihiko Ito, EnvInfoSci
Prof. Junji Shikata, EnvInfoSci
Prof. Masahiro Ishikawa, EnvInfoSci
Assoc. Prof. Shinji Yamamoto, EnvInfoSci
Assoc. Prof. Taro Arakawa, Eng.
Assoc. Prof. Junji Fukuda, Eng.
Assoc. Prof. Tadashi Nittami, Eng.
Prof. Yasumi Kawamura, Eng.
Prof. Junichi Okabe, Intern. Social Sci.

Acknowledgement

This Program was financed by one of the YNU priority funds for providing cooperation strategically and effectively and the special fund at YNU leading to development of international collaboration. The contents of the Program were planned by the organizing committee at YNU, and conducted by cooperation of many volunteers at YNU and City of Yokohama, Companies, and Materials & Surface Engineering Research Institute, Kanto Gakuin University. Sincere gratitude to the volunteers is offered for their warm support.


横濱
波止場ヨリ
海岸通
異人舘之
真圖