# International mini-symposium on advanced materials

**July 27, 2018**

**Host： Polymer・Hybrid Materials Research Center (PHyM)**

**Co-host：Nano-Macro Materials, Devices and System Research Alliance**

**Network Joint Research Center for Materials and Devices**

**Venue: Large meeting room, Administration Building 2F, Katahira campus, Tohoku University**

**Admission: Free**

## Program

14:00- 14:55 Invited talk: **Prof. Yoong Ahm Kim (Chonnam National University)**
"Linear Carbon Chains inside Carbon Nanotubes"

15:00- 15:55 Invited talk: **Prof. George Shimizu (University of Calgary)**
"$CO_2$ Capture and Proton Conduction in Metal Organic Frameworks"

16:00- 16:40 Invited talk: **Dr Biplab Joarder (Kyushu University)**
"Design, Synthesis and Functional Studies of Coordination Polymers"

### *Special event: Doctoral student course "Global Research Skill Training Dojo"*

10:20- 11:20 @ Kyotani laboratory

***International Advisor: Prof. Yoong Ahm Kim***

Rui Tang, "Understanding the origin of carbon anodic oxidation in supercapacitors from a molecular point of view"

Keita Nomura, "Nanoporous electrodes consisting of edge-free graphene walls for extraordinarily stable supercapacitors"

16:40- 17:40 @ Large meeting room, Administration Building 2F

***International Advisor: Prof. George Shimizu and Dr Biplab Joarder***

Ayumi Kawasaki, "Electron transport properties and molecular assemblies of ion-pair n-type semiconductor"

Wu JianYun, "Solid state ferroelectricity derived from bowl-shaped trithiasumanene derivatives"

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# Linear Carbon Chains inside Carbon Nanotubes

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The fascinating ability of a carbon atom to bind itself via different hybridization states (sp, $sp^2$ and $sp^3$) has generated a wide range of carbon allotropes. Two examples of natural carbon allotropes are diamond (with three-dimensional $sp^3$-hybridized carbon atoms) and graphite (with two dimensional sp2-hybridized carbon atoms). Additional $sp^2$-basd carbon allotropes, such as fullerene, carbon nanotube and graphene have contributed to development of carbon science and technology at the nanoscale. A third type of carbon allotrope is linear carbon chain (called LCCs) which comprises sp-hybridized carbon. LCCs are expected to exhibit stronger mechanical strength than diamond and its higher electron mobility than graphene and carbon nanotubes. However, there is a large difficulty in handing LCCs due to their extremely high chemical reactivity including the explosiveness. Currently, they can be stabilized by attaching giant molecules on the end sites and by encasing them in the hollow core of various carbon nanotubes (CNTs). Even though the experimental evidence on the presence of LCCs inside CNTs using transmission electron microscope and Raman tools was reported earlier, there are many questions to be answered; (a) how they grow inside CNTs, (2) how much they are structurally and thermally stable with regard to high temperature thermal treatment and/or boron doping process and (3) how do they contribute to the electrical properties of CNTs. In this talk, the current status of recent research on the synthesis and characterizations of linear carbon chains will be discussed, especially by focusing on infinite linear carbon chains [1, 2].

[1] C.-S. Kang, K. Fujisawa, Y.-I. Ko, H. Muramatsu, T. Hayashi, M. Endo, H. J. Kim, D. Lim, J. H. Kim, Y. C. Jung, M. Terrones, M. S. Dresselhaus, Y. A. Kim, Carbon, 107, 217 (2016)
[2] A. Bianco, Y. Chen, Y. Chen, D. Ghoshal, R. H. Hurt, Y. A. Kim, N. Koratkar, V. Meunier, M. Terrones, Carbon, 132, 785 (2018).

# $CO_2$ Capture and Proton Conduction in Metal Organic Frameworks

George Shimizu

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Key words: MOFs, carbon dioxide capture, proton conduction

**Abstract**

Metal organic frameworks (MOFs) represent tunable molecular scaffoldings that can be adjusted for a breadth of applications. This presentation will concern our efforts towards tailoring MOFs towards two globally relevant energy challenges, $CO_2$ capture and fuel cells.

The first topic concerns MOFs as proton conductors.[1] In this light, MOFs offer several interesting prospects stemming from their modular syntheses and tunable pore structures. MOFs have been shown to be able to conduct protons over $10^{-1}$ $Scm^{-1}$,[2] conduct above the boiling point of water,[3] and also to be robust in humid atmospheres[4] – an ongoing challenge is to merge all desirable properties in one material. Even when the properties of the MOF may not meet a required industrial standard, the crystallinity of the MOF can allow for added insights to designing better materials and as a foothold for modelling studies.[5] This aspect of the talk will cover some recent work to fine tune proton conduction but also efforts to make robust materials.

For the carbon capture portion, the talk will concern the factors that both make a solid an academically interesting capture material and also those that carry forward to more practical application. In contrast to liquid amines which chemisorb $CO_2$ and have high energy costs for regeneration, the MOF approach typically gives physisorbed gases and hence more facile release.[6] This topic will cover factors affecting CO2 affinity in MOFs.[7] Finally, we will present a new MOF with high stability that can capture $CO_2$ via a physisorptive mechanism in wet gas.[8] This material has been patented and the commercialization path will also be discussed.

**Reference:**

1. a) Yamada, T. et al. Bull. Chem. Soc. Jpn.2016, 89, 1-10. b) Sadakiyo, M. et al. CHEMPLUSCHEM, 2016, 81 691-701. c) G. K. H. Shimizu et al. *Science*, **2013**, *341*, 354.

2. a) Ramaswamy, P. et al. *J. Am. Chem. Soc*. **2015**, *137*, 7640.b) S. Kim et al., *J. Am. Chem. Soc.* **2018***, 140,* 1077.

3. a) J. A. Hurd et al. *Nature Chem*. **2009**, *1*, 705. b) Bureekaew, S. et al. *Nature Mater.* **2009**, *8*, 831. c) Inukai, M. et al. *J. Am. Chem. Soc.* **2016***, 138,* 8505.

4. a) J. M. Taylor et al., *J. Am. Chem. Soc.* **2013***, 135,* 1193. b) N. Wong et al. *J. Am. Chem. Soc.* **2017***, 139,* 14676

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6. a) Sumida, K. et al. *Chem Rev*. **2012**, 112, 724. b) Patel, H. A. et al, CHEMSUSCHEM, **2017**, DOI: **10.1002/cssc.201601545**

7. a) R. Vaidhyanathan et al. *Science,* **2010**, *330*, 650. b) Gelfand, B. S. et al *Angew. Chem. Int. Ed.* **2016**, 55,14614.

8. Shimizu, G. K. H. US, AUS patent awarded.

**Design, Synthesis and Functional Studies of Coordination Polymers**

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**Abstract**

The ubiquitous influence of porous materials has been a key factor for making the new-generation materials indispensable in life for a long time.[1] Among all the porous materials, the class of coordination polymers (CPs) based porous materials has emerged as the one of the promising candidate for the targeted applications over the last decade. CPs are solid crystalline materials constituted via self-assembly of single metal cations (primary building unit or PBU) or metal clusters (secondary building unit or SBU) and organic linkers containing multiple binding sites, in order to form one, two, or three dimensional extended coordination networks.[2] The inherent long-range order omnipresent in these substances coupled with the unique tunable nature consequently reflects in a commanding influence on their functional behavior during comprehensive investigation of different application-oriented phenomena. This lecture will be on development of functionalized CP materials for hydrocarbon separation,[3] explosive sensing[4] and proton conduction application[5].

**Reference:**

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2. (a) Moulton, B.; Zaworotko, M. J. *Chem. Rev.* **2001**, *101*, 1629; (b) Yaghi, O. M.; O'Keeffe, M.; Ockwig, N. W.; Chae, H. K.; Eddaoudi, M.; Kim, J. *Nature* **2003**, *423*, 705.
3. Joarder, B.; Mukherjee, S.; Chaudhari, A. K.; Desai, A. V.; Manna, B.; Ghosh, S. K. *Chem.-Eur. J.* **2014**, *20*, 15303
4. Joarder, B.; Desai, A. V.; Samanta, P.; Mukherjee, S.; Ghosh, S. K. *Chem.-Eur. J.* **2015**, *21*, 965
5. Joarder, B.; Lin, J.-B.; Romero, Z.; Shimizu, G. K. H. *J. Am. Chem. Soc.* **2017**, *139*, 7176.