Organized by Endorsed by
8th IUPAC INTERNATIONAL CONFERENCE ON GREEN CHEMISTRY
9 - 14 September 2018, Shangri-La Hotel, Bangkok, Thailand

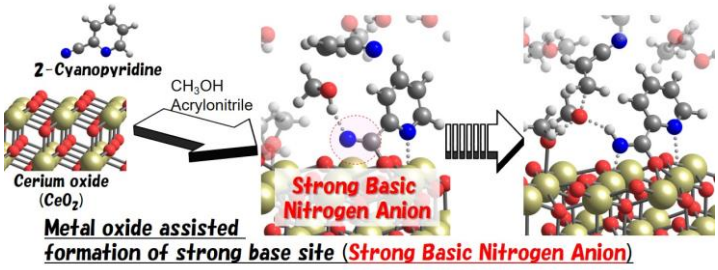
8th ICGC 2018 Session:

Catalytic reactions at the liquid/metal-oxide interface: first-principle molecular dynamics simulation

Akira Nakayama[1,2*]
[1]*Institute for Catalysis, Hokkaido University, Sapporo 001-0021, Japan*
[2]*JST PRESTO, Japan*
*e-mail: nakayama@cat.hokudai.ac.jp

Abstract:

A detailed understanding of the interface between liquid and metal-oxide is fundamental due to its relevance to the broad range of physicochemical phenomena and technological applications. Chemical reactions occurring at the liquid/metal-oxide interface are very complex, and the probing of the microscopic nature of the interface remains a formidable task for experiments. In this work, by employing the first-principles molecular dynamics simulations, we focus on the catalytic reactions at the water/CeO_2 and methanol/CeO_2 interface and investigate the role of acid-base and redox sites over CeO_2. We will present the following topics: (1) Structure and dynamical properties of water molecules at the water/CeO_2 and water/ZrO_2 interfaces. (2) Substrate-specific adsorption of 2-cyanopyridine and hydration reaction over CeO_2 explored by the free energy landscape with the aid of metadynamics simulations. (3) Self-assembled hybrid catalysis of 2-cynopyridine and CeO_2 and a formation of strong base site by hybridization. (4) The reaction mechanism for the direct synthesis of dimethyl carbonate (DMC) from methanol and CO_2 over CeO_2 and ZrO_2.



References: (if applicable)

1. Tamura, M.; Kishi, R.; Nakayama, A.; Nakagawa, Y.; Hasegawa, J.; Tomishige, K. *J. Am. Chem. Soc.* **2017**, *139*, 11857.
2. Nakayama, A.; Tamura, M.; Shimizu, K.; Hasegawa, J. (in preparation)

1996 Bachelor of Engineering, Department of Applied Chemistry, School of Engineering, University of Tokyo; 2001 Ph.D., Department of Chemical System Engineering, Graduate School of Engineering, University of Tokyo; 2001-2005 Postdoctoral Research Associate, Department of Chemistry, University of Illinois at Urbana-Champaign; 2005-2013 Assistant Professor, Department of Chemistry, Faculty of Science, Hokkaido University; 2013-2015 Associate Professor, Catalysis Research Center, Hokkaido University; 2015-present Associate Professor, Institute for Catalysis, Hokkaido University; 2016-present PRESTO Researcher, JST
Research fields: theoretical chemistry, catalysis, photochemistry, quantum simulation