Yuki Sakamoto

Wako-city, Saitama, Japan

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EDUCATION

Ph.D. in Science **March 2018**

Tokyo Institute of Technology, Tokyo, Japan

Dissertation title: "Theoretical Study of the Electrocatalyst Materials for the Highly Efficient Water Decomposition and Oxygen Evolution Reaction"

Advisor: Dr. Shinichiro Nakamura, Head of Nakamura Laboratory, RIKEN, Japan

M.S. in Science **March 2015**

Tokyo Institute of Technology, Tokyo, Japan

B.S. in Science **March 2013**

Tokyo Institute of Technology, Tokyo, Japan

RESEARCH EXPERIENCE

Nakamura Laboratory, RIKEN, Saitama, Japan **2019-Present**

- Computational study of electrochemical process of CO_2 activation

Mitsubishi Chemical Corporation, Kagawa, Japan **2018-2019**

- Evaluation of the plant capacity by process simulations
- Performed chemical analyses of industrial process

Nakamura Laboratory, RIKEN, Saitama, Japan **2015-2018**

As a Ph.D. course student trainee from Tokyo Institute of Technology

- Theoretical study of the physical properties of electrocatalysts for artificial photosynthesis
- Revealed the characteristic electronic structures of the highly efficient 3d-metal based electrocatalysts
- Collaborative study of the crystal structures and solvation process of functional molecules
- Performed electronic structure calculations and classical molecular dynamics (MD) calculations using the super computers

Tachibana Laboratory, Tokyo Institute of Technology, Tokyo, Japan **2012-2015**

B.S. and M.S. study

- Biochemical study of the control mechanism of the initiation of DNA replication
- Found protein elements which is essential for the initiation of DNA replication

- Performed biochemical experiments: PCR, western blot, and inhibitor experiments etc.

RESEARCH SKILLS

- Molecular science: Quantum chemical calculations
- Solid state chemistry: First principles band structure calculations
- Numerical analysis and scientific programing

PUBLICATIONS

- **Yuki Sakamoto**, Yusuke Noda, Kaoru Ohno, and Shinichiro Nakamura, "Chemical Insights from Theoretical Electronic States in Nickel Hydroxide and Monolayer Surface Model" *J. Phys. Chem. C.*, 2017, 121(44), pp 24603-24611
- Makoto Hatakeyama, **Yuki Sakamoto**, Koji Ogata, Yuto Sumida, Tomoe Sumida, Takamitsu Hosoya and Shinichiro Nakamura "A study on an unusual SN_2 mechanism in the methylation of benzyne through nickel-complexation", *Phys. Chem. Chem. Phys.*, 2017, 19, 26926-26933
- Kazuto Ikemoto, **Yuki Sakamoto**, Rikako Tanaka, Koji Ogata, Nobuyuki Matsushita, and Shinichiro Nakamura, "Unusual Ionic Bond and Solubility Mechanism of Na_nPQQ (n = 0–4) Crystals", *Cryst. Growth. Des.*, 2017, 17 (8), pp 4118–4123
- **Yuki Sakamoto,** Yusuke Noda, Kaoru Ohno, Kayo Koike, Katsushi Fujii, Tomiko Suzuki, Takeshi Morikawa, Shinichiro Nakamura “First Principles Calculation of Surface Dependent Electronic Structures: A Study on β-FeOOH and γ-FeOOH”, *Phys. Chem. Chem. Phys.,* in press (2019)
- Koji Ogata, Makoto Hatakeyama, **Yuki Sakamoto**, Shinichiro Nakamura “Investigation of Pathway for Water Delivery in Photosystem II Protein by Molecular Dynamics Simulation”, *J. Phys. Chem. B.*, in press (2019)

(In Japanese)

- Kazuto Ikemoto, **Yuki Sakamoto**, Kumiko Horiguchi, Shinichiro Nakamura, “^{13}C-NMR Measurement of Pyrroloquinoline Quinone in Deuterium Oxide Using Cryo-probe and Spectral Identification by the Quantum Chemical Calculation”, BUNSEKI KAGAKU, 2018, 67 (4), pp195-199

CONFERENCE PRESENTATIONS

- **Yuki Sakamoto**, Rikako Tanaka, Koji Ogata, Kazuto Ikemoto, Nobuyuki Matsushita, Shinichiro Nakamura “Theoretical study of PQQ, the rate of dissolution and equilibrium states in water”, 2016, The 96th CSJ (The Chemical Society of Japan) Annual Meeting, Doshisha Uniersity, Kyoto, Japan (March 2016)

- **Yuki Sakamoto**, Shinichiro Nakamura “First principles calculation of Nickel Hydroxide”, The 97th CSJ (The Chemical Society of Japan) Annual Meeting, Keio University, Yokohama, Japan (March 2017)
- **Yuki Sakamoto**, Shinichiro Nakamura, “The First Principles Study of Oxygen Evolving Reaction in β-FeOOH”, The 78th JSAP (The Japan Society of Applied Physics) Autumn Meeting, Fukuoka Convention Center, Fukuoka, Japan (September 2017)

CONTRIBUTING PROJECTS

- **E-Cell project**: Open source software environment for biochemical simulations, hosted by RIKEN, Japan. The codes are available on github.com.
- **HartreeFock_Solver**: (self-improvement project) A simple implementation of Hartree-Fock method, which is the basic algorithm of *ab initio* quantum chemistry methods.

HONORS AND AWARDS

- Junior Research Associate Program, RIKEN, 2017
- The scholarship loan program of JASSO (category 1 loans)
  I was released from the duty of 50% repayment as one of the highest-achievers in the Tokyo Institute of Technology.

COMPUTER SKILLS

- OS: Windows, UNIX, LINUX
- Programming: C/C++, Python, Ruby (more than 8 years)
- Computational chemistry software: Gaussian, Quantum ESPRESSO, ORCA