

Department of Chemistry

Research Area : Structural Chemistry

(URL : http://chem.okayama-u.ac.jp/~solid/index_e.html)

Hiroyuki ISHIDA, Professor

Kazuma GOTOH, Associate Professor

Research Themes :

- » Crystal engineering by use of intermolecular interactions
- » Structure and properties of porous solids and battery materials using nuclear magnetic resonance
- » Research and development of porous carbon materials

Representative Publication :

- R. Morita, K. Gotoh, M. Fukunishi, K. Kubota, S. Komaba, T. Yumura, N. Nishimura, K. Deguchi, S. Ohki, T. Shimizu and H. Ishida
Combination of solid state NMR and DFT calculation to elucidate the state of sodium in hard carbon electrodes *J. Mater. Chem. A*, **4**, 13183-13193 (2016).
- K. Gotoh, H. Maruyama, T. Miyatou, M. Mizuno, K. Urita, and H. Ishida
Structure and Dynamic Behavior of Na-Diglyme Complex in the Graphite Anode of Sodium Ion Battery by ²H Nuclear Magnetic Resonance *J. Phys. Chem. C*, **120**, 28152-28156 (2016).
- K. Gotoh and H. Ishida
Hydrogen-bonded structures of the 1:1 and 1:2 compounds of chloranilic acid with pyrrolidin-2-one and piperidin-2-one *Acta Cryst. C* **67**, o500–o504 (2011).

Research Area : Molecular Spectroscopy

(URL : http://chem1.chem.okayama-u.ac.jp/~spectro/home_en3.htm)

Jian TANG, Professor

Research Themes:

- » High-resolution spectroscopy of free radicals and molecular ions
- » Infrared spectroscopy of molecular clusters
- » Spectroscopic and reaction dynamics studies of interstellar molecules
- » Non-linear Spectroscopy

Representative Publication :

- K. Kawaguchi, R. Fujimori, J. Tang, and T. Ishiwata
FTIR Spectroscopy of NO₃ : Perturbation Analysis of the $\nu_3+\nu_4$ State *J. Phys. Chem. A* **117**, 13732–13742 (2013).
- Y. Miyamoto, H. Ooe, S. Kuma, K. Kawaguchi, K. Nakajima, I. Nakano, N. Sasao, J. Tang, T. Taniguchi, and M. Yoshimura
Spectroscopy of HF and HF containing clusters in solid parahydrogen *J. Phys. Chem. A* **115**, 14254–14261 (2011).
- H. Ooe, Y. Miyamoto, S. Kuma, K. Kawaguchi, K. Nakajima, I. Nakano, N. Sasao, J. Tang, T. Taniguchi, M. Yoshimura
Diffusion of hydrogen fluoride in solid parahydrogen *J. Chem. Phys.* **138**, 214309-1-6 (2013).

Research Area : Synthetic and Physical Organic Chemistry

(URL: <http://chem.okayama-u.ac.jp/~spoc/index.html>)

Hideki OKAMOTO, Associate Professor

Research Themes:

- » Photochemical reactions and photophysical properties of cyclophanes
- » Synthesis of polycyclic aromatic compounds and their application to organic electronics
- » Development and photophysical properties of luminescent probes

Representative Publication :

- H. Okamoto, H. Takahashi, T. Takane, Y. Nishiyama, K. Kakiuchi, S. Gohda, and M. Yamaji, Convenient phenacene synthesis by sequentially performed Wittig reaction and Mallory photocyclization using continuous flow technique, *Synthesis*, **49**, pp. 2949–2957 (2017)
- H. Okamoto, T. Kozai, Z. Okabayashi, T. Shinmyozu, H. Ota, K. Amimoto, and K. Satake, Synthesis, structure, and photoreactions of fluorinated 2,11-diaza[3₂]paracyclophane: Photochemical formation of cage-diene type benzene dimer, *J. Phys. Org. Chem.*, **30**, e3726 (2017).
- M. Fujii, M. Namba, M. Yamaji and H. Okamoto, Solvent-induced multicolour fluorescence of amino-substituted 2,3-naphthalimides studied by fluorescence and transient absorption measurements, *Photochem. Photobiol. Sci.*, **15**, pp. 842–850 (2016). (Front cover article)

Research Area : Inorganic Chemistry

(URL: http://chem.okayama-u.ac.jp/~inorganic/index_eng.html)

Yasushige KURODA, Professor

Takahiro OHKUBO, Associate Professor

Research Themes:

- » Unprecedented states of metal-ions encapsulated in solid-inorganic compounds with nano-sized pores
- » Specific adsorption feature of metal-ion-exchanged zeolites
- » Confined structure of molecules and ions in carbon nanospace
- » New reactions using nano-carbons

Representative Publication :

- A. Oda, T. Ohkubo, T. Yumura, H. Kobayashi, and Y. Kuroda
Identification of stable Zn^{II}-oxyl species enforced by MFI and its reversible reactivity with O₂ at RT *Angew. Chem. Int. Ed.*, **56**, 9715–9718 (2017).
- A. Oda, T. Ohkubo, T. Yumura, H. Kobayashi, and Y. Kuroda
Why do zeolites induce unprecedented electronic state on exchanged metal ions? *Phys. Chem. Chem. Phys.*, **19**, 25105–25114 (2017).
- M. Nishi, T. Ohkubo, M. Yamasaki, H. Takagi, and Y. Kuroda
Surplus adsorption of bromide ion into p-conjugated carbon nanospaces assisted by proton coadsorption *J. Colloid Interface Sci.*, **508**, 415–418 (2017).

Research Area : Coordination Chemistry

(URL: <http://chem.okayama-u.ac.jp/~complex/Coord.Chem.Eng/Home.html>)

Takayoshi SUZUKI, Professor

Yukinari SUNATSUKI, Assistant Professor

Research Themes:

- » Synthesis of novel coordination compounds and control of their structures and functionalities
- » Complete spontaneous resolution of metal complexes
- » Synthesis and magnetic property of novel metal complexes



Representative Publication :

- A. Mori, T. Suzuki, Y. Nakatani, Y. Sunastuki, M. Kojima and K. Nakajima
Palladium(II) mononuclear and palladium(II)/ruthenium(II) heterodinuclear complexes containing 2-quinolyl-substituted (pyridine-2-carbonyl)hydrazone, *Dalton Trans.* **44**, 15757–15760 (2015).
- A. Kashima, M. Sakate, H. Ota, A. Fuyuhiko, Y. Sunatsuki and T. Suzuki
Thymine(2-)-bridged cyclic tetranuclear rhodium(III) complexes formed by a template of a sodium, calcium or lanthanoid ion, *Chem. Commun.* **51**, 1889–1892. (2015).
- T. Ueno, Y. Ii, T. Fujinami, N. Matsumoto, S. Iijima, and Y. Sunatsuki
Polymorphs of spin-crossover iron(II) complex *fac*-[Fe^{II}(HL^{*n*-Pr})₃]Cl · PF₆ (HL^{*n*-Pr} = 2-methylimidazol-4-yl-methylideneamino-*n*-propyl): Assembly structures and scan rate dependent spin-crossover properties with thermal hysteresis, *Polyhedron* **136**, 13–22 (2017).

Research Area : Molecular Surface Science

(URL: <http://interfa.rlss.okayama-u.ac.jp/index.html>)

Yoshihiro KUBOZONO, Professor
Hidenori GOTO, Associate Professor
Ritsuko EGUCHI, Assistant Professor

Research Themes:

- 》 Fabrication and characterization of superconductors of carbon-based materials and two-dimensional layered materials
- 》 Electronic devices (transistors) based on organic molecules and two-dimensional layered materials
- 》 Study on electronic properties of graphene and topological materials
- 》 Nanoscale science in light element materials

Representative Publication :

- R. Mitsuhashi, Y. Suzuki, Y. Yamanari, H. Mitamura, T. Kambe, N. Ikeda, H. Okamoto, A. Fujiwara, M. Yamaji, N. Kawasaki, Y. Maniwa, and Y. Kubozono, Superconductivity in alkali-metal-doped picene, *Nature* **464**, 76 (2010).
- H. Goto, E. Uesugi, R. Eguchi, A. Fujiwara, and Y. Kubozono, Edge-Dependent Transport Properties in Graphene, *Nano Lett.* **13**, 1126 (2013).
- M. Izumi, L. Zheng, Y. Sakai, H. Goto, M. Sakata, Y. Nakamoto, H. L. T. Nguyen, T. Kagayama, K. Shimizu, S. Araki, T. C. Kobayashi, T. Kambe, D. Gu, J. Guo, J. Liu, Y. Li, L. Sun, K. Prassides, and Y. Kubozono, Emergence of double-dome superconductivity in ammoniated metal-doped FeSe, *Sci. Rep.* **5**, 9477 (2015).

Research Area : Theoretical Physical Chemistry

(URL: <http://phys.chem.okayama-u.ac.jp/english/index.html>)

Kenichiro KOGA, Professor
Tomonari SUMI, Associate Professor

Research Themes:

- 》 Structure and phase transitions of liquids, liquid mixtures, and fluid interfaces
- 》 Hydrophobic effect
- 》 Development of density-functional theory for liquids and its application to thermodynamic stability of proteins
- 》 Stochastic modeling of molecular motors and biomolecular machines

Representative Publication :

- K. Koga, Osmotic Second Virial Coefficient of Methane in Water, *J. Phys. Chem. B* **117**, 12619 (2013).
- K. Mochizuki and K. Koga, Solid-liquid critical behavior of water in nanopores, *Proc. Natl. Acad. Sci. U.S.A.* **112**, 8221 (2015).
- I. Hatano, K. Mochizuki, T. Sumi, and K. Koga, Hydrophobic Polymer Chain in Water That Undergoes a Coil-to-Globule Transition Near Room Temperature, *J. Phys. Chem. B* **120**, 12127 (2016).
- T. Sumi, Y. Maruyama, A. Mitsutake, K. Mochizuki, and K. Koga, Application of reference-modified density functional theory: Temperature and pressure dependences of solvation free energy, *J. Comput. Chem.* **39**, 202 (2018).
- T. Sumi, Design principles governing chemomechanical coupling of kinesin, *Sci. Rep.* **7**, 1163 (2017).

Research Area : Physical Chemistry

(URL: <http://chem.okayama-u.ac.jp/english/staff/detail/yoshimi-sueishi.html>)

Yoshimi SUEISHI, Professor

Research Themes:

- » Multiple free-radical scavenging capacity of antioxidants in food, cosmetics and pharmaceuticals
- » Function control of inclusion materials based on complexation mechanism and its applications

Representative Publication :

- Y. Sueishi, E. Kamogawa, A. Kimura, G. Kitahara, H. Satoh, T. Asanuma, and S. Oowada
Multiple free-radical scavenging (MULTIS) capacity in cattle serum, *J. Clin. Biochem. Nutr.*, **60**, 76–80 (2017).
- Y. Sueishi, Y. Honda, S. Fujitani, N. Inazumi, and T. Hanaya
Investigation of inclusion complexation of imidazolium and pyrrolidinium chlorides with water-soluble p-sulfonatocalix[6]arene: characteristic effects of external pressure, temperature, and substituents, *J. Incl. Phenom. Macrocycl. Chem.*, **86**, 255–261 (2016).

Research Area : Theoretical Chemistry

(URL: <http://theochem.chem.okayama-u.ac.jp/english/index.html>)

Hideki TANAKA, Professor

Masakazu MATSUMOTO, Associate Professor

Research Themes:

- » Aquomics: a comprehensive study of water and hydrates
- » Theoretical study of the phase transitions and critical phenomena of water and hydrates
- » Crystal structure prediction of ices and hydrates
- » Structure and property of water and aqueous solutions in confined geometry

Representative Publication :

- K. Himoto, M. Matsumoto, and H. Tanaka, Yet another criticality of water, *Phys. Chem. Chem. Phys.* in press (2014). doi:10.1039/c3cp54726d.
- K. Mochizuki, M. Matsumoto, and I. Ohmine, Defect pair separation as the controlling step in homogeneous ice melting, *Nature* **498**, 350–354 (2013).
- H. Tanaka and M. Matsumoto, Statistical Mechanical Approach to the Thermodynamic Stability of Clathrate Hydrates, *Adv. Chem. Phys.* **152**, 421–462 (2013).

Research Area : Organic Chemistry

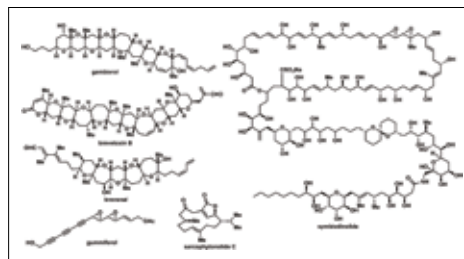
(URL: <http://chem.okayama-u.ac.jp/~organic/homeE.html>)

Isao KADOTA, Professor

Hiroyoshi TAKAMURA, Associate Professor

Research Themes:

- » Total synthesis of biologically active natural products
- » Development of new synthetic strategy and reaction
- » Structural elucidation of complex natural products based on chemical synthesis



Representative Publication :

- T. Tanaka, H. Asakura, R. Fujiwara, K. Kumamoto, H. Izuka, K. Shiroma, H. Takamura, and I. Kadota, Improved Synthesis of the A–E Ring Segment of Ciguatoxin CTX3C by Using Intramolecular Allylations, *Bull. Chem. Soc. Jpn.* doi:10.1246/bcsj.20170390 (2018).
- H. Takamura, T. Ohashi, T. Kikuchi, N. Endo, Y. Fukuda, and I. Kadota, Late-Stage Divergent Synthesis and Antifouling Activity of Geraniol–Butenolide Hybrid Molecules, *Org. Biomol. Chem.* **15**, pp. 5549–5555 (2017).
- H. Takamura, T. Fujiwara, Y. Kawakubo, I. Kadota, and D. Uemura, Stereodivergent Synthesis and Stereochemical Reassignment of the C79–C104 Fragment of Symbiodinolide, *Chem. Eur. J.* **22**, pp. 1984–1996 (2016).

Research Area : Organic Synthetic Chemistry

(URL: <http://chem.okayama-u.ac.jp/~orgsynth/index.html>)

Tadashi HANAYA, Professor

Research Themes:

- 》 Synthetic studies on natural pterin glycosides
- 》 Synthetic studies on sugar analogs having phosphorus in the ring and the related organophosphorus compounds

Representative Publication :

- T. Hanaya, K. Iwasaki, K. Saeki, and T. Hattori, Efficient Total Syntheses of Natural Neopterin Glycosides: Neopterin Glucuronide and Solfapterin, *Heterocycles*, **95**, 390-409 (2017).
- T. Hanaya and H. Yamamoto, Synthesis of Biopterin and Related Pterin Glycosides, *IUBMB Life*, **65**, 300-309 (2013).
- T. Hanaya, H. Baba, H. Toyota, and H. Yamamoto, Synthetic Studies on Pterin Glycosides: the First Synthesis of 2'-O-(α -D-Glucopyranosyl)biopterin, *Tetrahedron*, **65**, 7989-7997 (2009).

Research Area : Functional Organic Chemistry

(URL: <http://chem.okayama-u.ac.jp/~funcchem/english/index.html>)

Yasushi NISHIHARA, Professor

Masayuki IWASAKI, Assistant Professor

Hiroki MORI, Assistant Professor

Research Themes:

- 》 Synthesis of functional polycyclic aromatic compounds and its application to organic field-effect transistors
- 》 Development of the transition-metal catalyzed direct sulfurization reactions of the carbon-hydrogen bonds
- 》 The elucidation of reaction mechanisms using quantum chemical calculations
- 》 Synthesis of π -conjugated organic molecules directed towards organic thin film solar cells



Representative Publication :

- H. Mori, S. Hara, S. Nishinaga, and Y. Nishihara, Solar Cell Performance of Phenanthrothiophene-Isoindigo Copolymers Depends on Their Thin-Film Structure and Molecular Weight, *Macromolecules* **50**, pp. 4639-4648 (2017).
- Y. Kubozono, K. Hyodo, S. Hamao, Y. Shimo, H. Mori, and Y. Nishihara, Transistor Properties of 2,7-Dialkyl-Substituted Phenanthro[2,1-b:7,8-b']dithiophene, *Sci. Rep.* **6**, 38535 (2016).
- M. Iwasaki, T. Fujii, K. Nakajima, and Y. Nishihara, Iron-Induced Regio- and Stereoselective Addition of Sulfenyl Chlorides to Alkynes via a Radical Pathway, *Angew. Chem. Int. Ed.* **53**, pp. 13880-13884 (2014).

Research Area : Analytical Chemistr

(URL: http://chem.okayama-u.ac.jp/~analytical/home_e.html)

Takashi KANETA, Professor

Nobuyuki TAKEYASU, Associate Professor

Research Themes:

- 》 Analysis of single cells and single molecules
- 》 Development of nanomaterials and their application to analytical science

Representative Publication :

- K. Yamaguchi, N. Takeyasu and T. Kaneta, Determination of association constants between 5'-guanosine monophosphate gel and aromatic compounds by capillary electrophoresis, *Journal of Chromatography A*, **1288**, 149-154 (2013).
- G. Inoue, T. Kaneta, T. Takayanagi, J. Kakehi, H. Motose and T. Takahashi, Determination of polyamines in Arabidopsis thaliana by capillary electrophoresis using salicylaldehyde-5-sulfonate as a derivatizing reagent, *Analytical Methods* **5**, 2854-2859 (2013).
- A. Tabara and T. Kaneta. Discrimination of glycoproteins via two-color laser-induced fluorescence detection coupled with postcolumn derivatization in capillary electrophoresis. *Electrophoresis* **34**, 2316-2322 (2013).