Czech Society for the Properties of Water and Steam
Annual Report 2022

Submitted to IAPWS Executive Committee, November 2022

Steering board of CZPWS
Chair: Tomáš Němec (Institute of Thermomechanics of the Czech Academy of Sciences - IT CAS, nemec@it.cas.cz), Vice-Chair: Josef Šedlbauer (Technical University of Liberec), Secretary: Jan Hrubý (IT CAS), Member: Radim Mareš (University of West Bohemia), Member: Milan Sedlář (SIGMA Research and Development Institute).

CZPWS Meetings
Annual meeting of the CZPWS was held on June 15, 2022. The form of the meeting was hybrid. CZPWS members were informed about the activities of CZPWS Chair and approved CZPWS Financial Statements. Until 2021, payment of CZPWS Member Due to IAPWS was provided from a national grant led by T. Němec. This grant ended. CZPWS became a member of the Council of Scientific Societies of the Czech Republic (CSSCR). Member fee for 2022 and future CZPWS Member Dues to IAPWS will be paid based on the CZPWS membership in CSSCR. New steering board of CZPWS was elected for period 2023-2027: Jan Hrubý (chair), Milan Sedlář (vice-chair), Ondřej Bartoš (scientific secretary), Vladimír Majer (member), Adam Nový (member).

RESEARCH ACTIVITES
Calibration of vibrating tube densimeters using the IAPWS standards
Experimentalists from IT CAS in Prague continued in measurement of density of various fluids using accurate vibrating tube densimeteres (VTD). A calibration technique for highly sensitive commercial instrument Anton Paar DMA 5000 M operated at 0.1 MPa was developed based on the comparison with the IAPWS-95 equation of state for water and the IAPWS G8-10 guideline for humid air [1]. The uncertainty of the liquid density was thoroughly analyzed together with other aspects influencing the quality of obtained data such as the relation between fluid viscosity and damping, the isotopic composition of the calibration water, the measurement procedure covering VTD cleaning and filling, and the effect of water contained in samples. The high-pressure VTD Anton Paar DMA HP is currently being brought into operation [7]. Both densimeters are intended for accurate measurement of density of aqueous solutions.

Surface tension and vapor pressure of supercooled water
Recent work on surface tension of supercooled water at University of West Bohemia in Pilsen was reported by R. Mareš and J. Kalová [5]. J. Kalová also published a study of the vapor pressure of supercooled water [6].

Cavitation

The problems studied in the SIGMA Research and Development Institute and the Centre of Hydraulic Research in the period of June 2021 – June 2022 have been related mainly to the model-ling of cavitation erosion during the hydrodynamic cavitation and models of cavitation

instabilities. In cooperation with the Institute of Physics of the Czech Academy of Sciences, a new cavitation erosion stand has been used to test cavitation resistance of steel samples treated with LSP. In cooperation with the Moscow Power Engineering Institute, the Technical University of Liberec and the Wuhan University, the experimental and numerical modelling of unsteady cavitation phenomena in water has continued in the framework of internal grant projects. The experiments and numerical simulations have concentrated on the thermal effects of cavitation and on the in-fluence of surface hydrophobicity on cavitation phenomena [2]. The Centre of Hydraulic Research in cooperation with the Palacky University in Olomouc finished a new hot-water stand for testing high-performance pumps at the temperatures up to 190 °C, maximum pressure up to 40 bar and power input up to 11 MW. In cooperation with the Institute of Thermomechanics of the Czech Academy of Sciences and the Czech Technical University in Prague, experimental and numerical modelling of unsteady multiphase flow has continued, taking into account the interface of water and air [3], [4].

Publications

1. Prokopová O., Blahut A., Čenský M., Součková M., Vinš V.: Comments on temperature calibration and uncertainty estimate of the vibrating tube densimeter operated at atmospheric pressure, J. Chem. Thermodynamics 173 (2022) 106855.
2. Sedlář M., Komárek M., Šoukal J., Volkov A.V., Ryzhenkov A.V., Druzhinin A.A., Grigoriev S.V., Kachalin G.V, Kalakutskaya O.V.: Experimental and Numerical Studies into the Cavitation Impact of the Hydrofoil Surface with Different Treatments. Thermal Engineering, 69 (2022), 418-428. doi: 10.1134/S0040601522060064
3. Furst J., Halada T., Sedlář M., Krátký T., Procházka P., Komárek M.: Numerical analysis of flow phenomena in discharge object with siphon using lattice-Boltzmann method and CFD. Mathematics, 9 (2021), 1734. doi: 10.3390/math9151734
4. Uruba V., Procházka P., Sedlář M., Komárek M., Duda D.: Experimental and Numerical Study on Vortical Structures and their Dynamics in a Pump Sump. Water 2022, 14(13), 2039; doi.org/10.3390/w14132039
5. Kalová J., Mareš R., Temperature Dependence of the Surface Tension of Water, Including the Supercooled Region, Int. J. Thermophysics, 43, 10 (2022), doi.org/10.1007/s10765-022-03077-
6. Kalová J, Vapor Pressure of Supercooled Water, Int. J. Thermophysics, s (2022) 43: 165, doi.org/10.1007/s10765-022-03095-w

Conference Proceedings

7. Olga Prokopová, Miroslav Čenský, Aleš Blahut, Václav Vinš: *Design and testing of the supporting setup for the high-pressure vibrating tube densimeter*, EPJ Web of Conferences 264 (2022) 01033.

U.S. National Committee to IAPWS
2022 Report on Activities of Potential Interest to IAPWS
21 November 2022

Communicated from the Applied Chemicals and Materials Division, National Institute of Standards and Technology, Boulder, CO (Allan Harvey)**:**

In an IAPWS project, in collaboration with Marc Assael (Aristotle University, Greece) and Jan Sengers (University of Maryland and NIST), a new thermal conductivity formulation for heavy water was developed and approved as an IAPWS Release (IAPWS R18-21). The archival paper was published: M.L. Huber, R.A. Perkins, M.J. Assael, S.A. Monogenidou, R. Hellmann, and J.V. Sengers, "New International Formulation for the Thermal Conductivity of Heavy Water," *Journal of Physical and Chemical Reference Data* **51**, 013102 (2022).

A collaboration between NIST and the group of Prof. Tremaine at the University of Guelph has the objective of developing a standard formulation for the static dielectric constant of heavy water. Thus far, we have gathered the available data and made preliminary comparisons based on the existing H_2O correlation in order to see where there are gaps in the data that might need to be filled in based on H_2O behavior. It is hoped that a new formulation will be ready before the 2023 IAPWS meeting.

In December 2021, the History and Heritage Committee of ASME (American Society of Mechanical Engineers) designated "Standardized Steam Property Tables" as Historic Mechanical Engineering Landmark #276. This reflects the centennial of the ASME's efforts on standardized steam tables, which began in 1921. The accompanying brochure and other information are on the ASME website: https://www.asme.org/about-asme/engineering-history/landmarks/276-standardized-steam-property-tables.

Also in conjunction with the 100th anniversary of ASME steam tables efforts, a historical perspective article was published: A.H. Harvey and J.C. Bellows, "A Century of ASME Steam Tables," *Mechanical Engineering* **144**(1), 44 (2021/2022).

A review article has been prepared on the thermophysical properties of water, with an emphasis on IAPWS formulations: A.H. Harvey, J. Hrubý, and K. Meier, "Improved and Always Improving: Reference Formulations for Thermophysical Properties of Water," *Journal of Physical and Chemical Reference Data*, submitted (2022).

Communicated from the ASME Research and Technology Committee on Water and Steam in Thermal Systems (Bob Bartholomew)

The Water Technology Subcommittee has completed work on a new guideline, *Deaerator Performance Monitoring and Inspection Guideline*. This document is now available from ASME as an e-book for a nominal fee at https://asmedigitalcollection.asme.org/ebooks/book/291/Deaerator-Performance-Monitoring-and-Inspection.

Communicated from the Idaho National Laboratory *Center for Radiation Chemistry*, Idaho Falls, ID (Jacy Conrad)

Advancements in the Radiation Chemistry of Aqueous Systems

The *Idaho National Laboratory* (INL) Center for *Radiation Chemistry Research* (CR2) has provided significant fundamental insight into the radiation-induced behavior of various aqueous chemical systems relevant to the nuclear fuel cycle.

Elucidating the radiation-induced behavior of actinides in aqueous media
New insights were gained on the behavior of rare actinide ions in aqueous solutions of interest for the manipulation of actinide and nuclear fuel cycle materials. By employing novel electron pulse radiolysis techniques—utilizing the *Brookhaven National Laboratory* (BNL) *Laser Electron Accelerator Facility* (LEAF)—the INL CR2 measured the first-ever transient di- and tetra-valent californium and berkelium ion spectra and lifetimes, in addition to the associated kinetics arising from the reaction of the corresponding trivalent states with transient aqueous radiolysis products, specifically the hydrated electron (e_{aq}^-), hydrogen atom ($H^\bullet$), and hydroxyl radical ($^\bullet OH$) from water radiolysis. The lifetimes of these non-traditional late actinide oxidation states are of the order of microseconds, which is more than sufficient to influence the chemistry of their immediate (coordination sphere) and surrounding (bulk aqueous solution) environments. This work was funded by the U.S. Department of Energy (DOE) Office of Science, Office of Basic Energy Sciences, under Award DESC0021372, and published in the following paper:

- G.P. Horne, B.M. Rotermund, T.S. Grimes, J.M. Sperling, D.S. Meeker, P.R. Zalupski, N. Beck, D. Gomez Martinez, A. Beshay, D.R. Peterman, B.H. Layne, J. Johnson, A.R. Cook, T.E. Albrecht-Schönzart, and S.P. Mezyk, Transient Radiation-Induced Berkelium(III) and Californium(III) Redox Chemistry in Aqueous Solution. Inorganic Chemistry, **2022**, 61 (28), 10822, DOI: https://doi.org/10.1021/acs.inorgchem.2c01106.

Kinetics measured for the radiation-induced reduction of aqueous hexavalent chromium ions to 325 °C
Highly toxic hexavalent chromium [Cr(VI)] is found in industrial wastewaters, including those from nuclear power plants, as a leachate from stainless steels. Electron pulse radiolysis using the *Notre Dame Radiation Laboratory* (NDRL) *Linear Accelerator* (LINAC) was employed to measure chemical kinetics and Arrhenius parameters for the reactions of Cr(VI) with water radiolysis products to 325 °C. It was determined that Cr(VI) is reduced to Cr(III) under irradiation, however, the oxidation between Cr(V) and the $^\bullet OH$ radical needs to be suppressed for complete reduction to occur. These new findings can be incorporated into models of chromium speciation under the extreme conditions present in operating nuclear reactors. The results of this work, funded by the INL Laboratory Research & Development (LDRD) Program under the U.S. Department of Energy (DOE) Idaho Operations Office Contract DE-AC07-05ID14517 have been published in the following paper:

- J.K Conrad, A. Lisouskaya, D.M. Bartels, Pulse Radiolysis and Transient Absorption of Aqueous Cr(VI) Solutions up to 325 °C. ACS Omega, **2022**, 7(43), 39071-39077, DOI: https://doi.org/10.1021/acsomega.2c04807.

Predictive multiscale model for the degradation pathways of acetohydroxamic acid in aqueous solutions under irradiation
Acetohydroxamic acid (AHA) has been proposed for use in used nuclear fuel reprocessing flowsheets for the reduction and complexation of plutonium and neptunium ions. New reaction

kinetics were measured for the reactions of AHA with the primary radiolysis products of water and nitric acid solutions, including the e_{aq}^-, H• atom, •OH and nitrate (NO_3•) radicals, using electron pulse radiolysis at the BNL LEAF and the NDRL LINAC. Using these measured kinetic rate coefficients, a predictive multiscale computer model has been developed for the radical-induced behavior of AHA in acidic aqueous solutions. This model has been rigorously evaluated against steady-state irradiations performed using the INL CR2 cobalt-60 gamma irradiator. These findings give a complete picture of the degradation pathways of AHA under proposed used nuclear fuel reprocessing conditions. This work, funded by the U.S. Department of Energy Assistant Secretary for Nuclear Energy, Material Recovery and Waste Form Development Campaign yielded the recent publication:

- J.K Conrad, C.D. Pilgrim, S.M. Pimblott, S.P. Mezyk, G.P. and Horne, Multiscale Modelling of the Radical-Induced Chemistry of Acetohydroxamic Acid in Aqueous Solution. RSC Advances, **2022**, 12(46), 29757-29766. DOI: https://doi.org/10.1039/D2RA03392E.

Communicated from the University of Maryland, College Park (Jan Sengers)

The IAPWS project on the development of new formulations for the viscosity and thermal conductivity of H2O and D2O has now been completed with the publication of

"New international formulation for the thermal conductivity of heavy water", M.L. Huber, R.A. Perkins, M.J. Assael, S.A. Monogenidou, R. Hellmann, and J.V. Sengers, J. Phys. Chem. Ref. Data 51, 013102 (2022), 19pp. https://doi.org/10.1063/5.0084222.

Communicated from EPRI, Palo Alto, CA (Chuck Marks, Dominion Engineering)

Aqueous chemistry of boric acid and alkali borates at elevated temperature
In recent years EPRI has led a collaborative effort of participants from multiple countries in obtaining new data on speciation and volatility of boric acid at elevated temperatures, developing new models for the activity coefficients of boric acid species, and developing expressions for the equilibrium coefficients for relevant reactions at infinite dilution. The results of this work are being incorporated into EPRI's ChemWorks Tools / MULTEQ and BOA software for modeling of nuclear reactor coolant chemistry.

Re-evaluation of the water dissociation equilibrium at high temperatures
As part of the boric acid work discussed above, a comparison of calculations with ChemWorks Tools and OLI's software indicated that differences in the treatment of the dissociation of water contributed significantly more to uncertainty in high temperature chemistry calculations than uncertainty in the speciation of boric acid. Comparisons of the IAWPS formulation with legacy formulations (e.g., that of Marshall and Franck) had previously indicated comparable uncertainty, but few experimental data were available to reduce the uncertainty. EPRI has begun an evaluation of the new data developed by Arcis, et al. with the objective of developing a new expression for the ionization of water at elevated temperatures.

Current Status of Research Activities in Japan
Submitted to the Executive Committee Meeting, IAPWS,
December, 2022

Japanese National Committee, Chaired by Professor Kenji Yasuoka
International Association for the Properties of Water and Steam
c/o The Japan Association for the Properties of Water and Steam
Chaired by Professor Kenji Yasuoka
3-14-1 Hiyoshi, Kohoku-ku,
Yokohama 223-8522, Japan

I. Overview:

The Japan National Committee of IAPWS continues to endeavor to make closer and innovative interactions between engineering and academic groups with respect to the international and domestic energy-related issues. The key points of our attention are cleaner, greener, and more sustainable energy as well as high efficiency and safety. We are discussing the science and engineering of fuels, boilers, turbines, and water-treatment. Now we take it into account the power generation from geothermal and biomass energies. Our activities in the publication are shown below.

II. Recent Publications:

Yasuoka, Kenji
Professor, Department of Mechanical Engineering, Keio University
email: yasuoka@mech.keio.ac.jp
URL: https://k-ris.keio.ac.jp/html/100011311_en.html

Correlation between ordering and shear thinning in confined OMCTS liquids
Y. Kobayashi, N. Arai, K. Yasuoka
J. Chem. Phys., 157, 114506 (10 pages), 2022

Impact of free energy of polymers on polymorphism of polymer-grafted nanoparticles
M. Ishiyama, K. Yasuoka, M. Asai
Soft Matter, 18, 6318-6325, 2022

Optimal Replica-Exchange Molecular Simulations in Combination with Evolution Strategies
A. Kowaguchi, K. Endo, P. E. Brumby, K. Nomura, K. Yasuoka
J. Chem. Inf. Model., DOI: 10.1021/acs.jcim.2c00608

Differences in ligand-induced protein dynamics extracted from an unsupervised deep learning approach correlate with protein–ligand binding affinities
I. Yasuda, K. Endo, E. Yamamoto, Y. Hirano, K. Yasuoka
Commun. Biol., 5, 481 (9 pages), 2022

A stochastic Hamiltonian formulation applied to dissipative particle dynamics
L. Peng, N. Arai, K. Yasuoka
Appl. Math. Compu., 426, 127126 (13 pages), 2022

Efficient Monte Carlo Sampling for Molecular Systems Using Continuous Normalizing Flow
K. Endo, D. Yuhara, K. Yasuoka
J. Chem. Theory Comput., 18, 1395-1405, 2022

Natural quantum reservoir computing for temporal information processing
Y. Suzuki, Q Gao, K. C. Pradel, K. Yasuoka, N. Yamamoto
Sci. Rep., 12, 1353 (15 pages), 2022

An Efficient Random Number Generation Method for Molecular Simulation
K. Okada, P. E. Brumby, K. Yasuoka
J. Chem. Inf. Model., 62, 71-78, 2022

Water molecules in CNT–Si3N4 membrane: Properties and the separation effect for water–alcohol solution
Winarto, E. Yamamoto, K. Yasuoka
J. Chem. Phys., 155, 104701 (11 pages), 2021

On effective radii of dodecahedral cages in semiclathrate hydrates for van der Waals and Platteeuw model
S. Muromachi, S. Takeya, D. Yuhara, K. Yasuoka
Fluid Phase Equil., 527, 112846 (6 pages), 2021

The influence of random number generation in dissipative particle dynamics simulations using a cryptographic hash function
K. Okada, P.E. Brumby, K. Yasuoka
PLoS ONE, 16, e0250593 (8 pages), 2021

Phase Transitions and Hysteresis for a Simple Model Liquid Crystal by Replica-Exchange Monte Carlo Simulations
A. Kowaguchi, P. E. Brumby, K. Yasuoka
Molecules, 26, 1421 (14 pages), 2021

Matubayasi, Nobuyuki
Professor, Graduate School of Engineering Science, Osaka University
email: nobuyuki@cheng.es.osaka-u.ac.jp
URL: http://www.cheng.es.osaka-u.ac.jp/matubayasi/english/index.html

Molecular dynamics study of the interactions between a hydrophilic polymer brush on graphene and amino acid side chain analogues in water
T. Yagasaki, N. Matubayasi
Phys. Chem. Chem. Phys., 24, 22877-22888, 2022

Constructing a Memory Kernel of the Returning Probability to Efficiently Describe Molecular Binding Processes
K. Kasahara, R. Masayama, Y. Matsubara, N. Matubayasi
Chem. Lett., 51, 823-827, 2022

Crystal Growth of Urea and Its Modulation by Additives as Analyzed by All-Atom MD Simulation and Solution Theory
S. Tanaka, N. Yamamoto, K. Kasahara, Y. Ishii, N. Matubayasi
J. Phys. Chem. B, 126, 5274-5290, 2022

Surface Area Estimation: Replacing the Brunauer-Emmett-Teller Model with the Statistical Thermodynamic Fluctuation Theory
S. Shimizu, N. Matubayasi
Langmuir, 38, 7989-8002, 2022

Nonpolarizable Force Fields through the Self-Consistent Modeling Scheme with MD and DFT Methods: From Ionic Liquids to Self-Assembled Ionic Liquid Crystals
Y. Ishii, N. Matubayasi, H. Washizu
J. Phys. Chem. B, 126, 4611-4622, 2022

Adsorption Energetics of Amino Acid Analogs on Polymer/Water Interfaces Studied by All-Atom Molecular Dynamics Simulation and a Theory of Solutions
N. Yasoshima, T. Ishiyama, N. Matubayasi
J. Phys. Chem. B, 126, 4389-4400, 2022

All-atom molecular simulation study of cellulose acetate: amorphous structure and the dissolution of small molecule
R. Matsuba, H. Kubota, N. Matubayasi
Cellulose, 29, 5463-5478, 2022

Explaining reaction coordinates of alanine dipeptide isomerization obtained from deep neural networks using Explainable Artificial Intelligence (XAI)
T. Kikutsuji, Y. Mori, K. Okazaki, T. Mori, K. Kim, N. Matubayasi
J. Chem. Phys., 156, 154108 (8 pages), 2022

Anion-cation contrast of small molecule solvation in salt solutions
S. Hervø-Hansen, J. Heyda, M. Lund, N. Matubayasi
Phys. Chem. Chem. Phys., 24, 3238-3249, 2022

Simulating the nematic-isotropic phase transition of liquid crystal model via generalized replica-exchange method
K. Takemoto, Y. Ishii, H. Washizu, K. Kim, N. Matubayasi
J. Chem. Phys., 156, 014901 (8 pages), 2022

Ensemble transformation in the fluctuation theory
S. Shimizu, N. Matubayasi
Physica A, 585, 126430 (14 pages), 2022; Physica A, 605, 127987 (1 pages), 2022

Molecular Structure and Vibrational Spectra of Water Molecules Sorbed in Poly(2-methoxyethylacrylate) Revealed by Molecular Dynamics Simulation
N. Yasoshima, T. Ishiyama, M. Gemmei-Ide, N. Matubayasi
J. Chem. Phys B, 125, 12095-12103, 2021

Atomistic description of molecular binding processes based on returning probability theory
K. Kasahara, R. Masayama, K. Okita, N. Matubayasi
J. Chem. Phys., 155, 204503 (15 pages) 2021

Effects of chain length on Rouse modes and non-Gaussianity in linear and ring polymer melts
S. Goto, K. Kim, N. Matubayasi
J. Chem. Phys., 155, 124901 (10 pages), 2021

Crystallization of Polyethylene Brushes and Its Effect on Interactions with Water
T. Yagasaki, N. Matubayasi
Macromolecules, 54, 8303-8313, 2021

Temperature Dependence of Sorption
S. Shimizu, N. Matubayasi
Langmuir, 37, 11008-11017, 2021

Breakdown of the Stokes-Einstein relation in supercooled liquids: a cage-jump perspective
R. Pastore, T. Kikutsuji, F. Rusciano, N. Matubayasi, K. Kim, F. Greco
J. Chem. Phys., 155, 114503 (7 pages), 2021

Cooperative Sorption on Porous Materials
S. Shimizu, N. Matubayasi
Langmuir, 37, 10279-10290, 2021

Water Dissolved in a Variety of Polymers Studied by Molecular Dynamics Simulation and a Theory of Solutions
H. Kojima, K. Handa, K. Yamada, N. Matubayasi
J. Phys. Chem. B, 125, 9357-9371, 2021

Molecular insights on confined water in the nanochannels of self-assembled ionic liquid crystal
Y. Ishii, N. Matubayasi, G. Watanabe, T. Kato, H. Washizu
Sci. Adv., 7, eabf0669 (14 pages), 2021

Construction of isostructural hydrogen-bonded organic frameworks: limitations and possibilities of pore expansion
Y. Suzuki, M. Gutiérrez, S. Tanaka, E. Gomez, N. Tohnai, N. Yasuda, N. Matubayasi, A. Douhal, I. Hisaki
Chem. Sci., 12, 9607-9618, 2021

Adsorbate-adsorbate interactions on microporous materials
S. Shimizu, N. Matubayasi
Micropor. Mesopor. Mater., 323, 111254 (8 pages), 2021

Sorption: A Statistical Thermodynamic Fluctuation Theory
S. Shimizu, N. Matubayasi
Langmuir, 37, 7380-7391, 2021
Transition pathway of hydrogen bond switching in supercooled water analyzed by the Markov state model
T. Kikutsuji, K. Kim, N. Matubayasi
J. Chem. Phys., 154, 234501 (7 pages), 2021

Understanding the scaling of boson peak through insensitivity of elastic heterogeneity to bending rigidity in polymer glasses
N. Tomoshige, S. Goto, H. Mizuno, T. Mori, K. Kim, N. Matubayasi
J. Phys.: Condens. Matter, 33, 274002 (7 pages), 2021

Cooperativity in micellar solubilization
S. Shimizu, N. Matubayasi
Phys. Chem. Chem. Phys., 23, 8705-8716, 2021

Spatial-Decomposition Analysis of Electrical Conductivity in Mixtures of Ionic Liquid and Sodium Salt for Sodium-Ion Battery Electrolytes
L. Hakim, Y. Ishii, N. Matubayasi
J. Phys. Chem. B, 125, 3374-3385, 2021

Implicit function theorem and Jacobians in solvation and adsorption
S. Shimizu, N. Matubayasi
Physica A, 570, 125801 (11 pages), 2021

Phase stability condition and liquid-liquid phase separation under mesoscale confinement
S. Shimizu, N. Matubayasi.
Physica A, 563, 125385 (13 pages), 2021

Solvation energetics of protein and its aggregates analyzed by all-atom molecular dynamics simulation and the energy-representation theory of solvation
N. Matubayasi
Chem. Comm., 57, 9968-9978, 2021

All-Atom Analysis of Partitioning Functions of Molecular Aggregates through Development of a Statistical-Mechanical Theory of Solutions
N. Matubayasi
Manuf. & Technol., 73, 61-64, 2021 (in Japanese)

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Evaluation of estimation accuracy of saturated properties and theoretical performance for refrigerants with ECS model
R. Teraishi, Y. Kayukawa, R. Akasaka, J. Jeong, K. Saito
Trans. Jpn. Soc. Refrig. Air Cond. Eng., 38, 196-205, 2021 (in Japanese).
Universal Parameters of the Extended Corresponding States (ECS) Model for Hydrofluoroolefin Refrigerants
R. Teraishi, Y. Kayukawa, R. Akasaka, K. Saito
Int. J. Refrig., 131, 33-40, 2021

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URL: http://pub2.db.tokushima-u.ac.jp/ERD/person/189117/work-en.html

Significant role of counterion for lead(II) ion adsorption on carbon pore surface
T. Horikawa, M. Okamoto, A. Kuroki-Matsumoto, K. Yoshida
Carbon, 196, 575-588, 2022

Structure and Formation Mechanism of Protective Coatings on Steam Piping Composed of Film-Forming Amines
K. Yoshida
The Thermal and Nuclear Power, 73, 32-39, 2022 (in Japanese)

Microscopic Structure and Binding Mechanism of the Corrosion-Protective Film of Oleylpropanediamine on Copper in Hot Water
H. Yoshioka, K. Yoshida, N. Noguchi, T. Ueki, K. Murai, K. Watanabe, M. Nakahara
J. Phys. Chem. C, 126, 6436-6447, 2022

Temperature dependence of water cluster on functionalized graphite
T. Horikawa, R. Yuasa, K. Yoshida, D. D. Do
Carbon, 183, 380-389, 2021

Solvation shell dynamics of supercritical water-cyclohexane mixtures in relation to the translational and rotational dynamics as studied by molecular dynamics simulation
K. Yoshida, H. Yoshioka
AIP Advances, 11, 075219 (12 pages), 2021

^{14}N NMR Evidence for Initial Production of NH_3 Accompanied by Alcohol from the Hydrolysis of Ethylamine and Butylamine in Supercritical Water
K. Yoshida, H. Yoshioka, N. Ushigusa, M. Nakahara
Chem. Lett, 50, 316-319, 2021

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Microscopic Structure and Binding Mechanism of the Corrosion-Protective Film of Oleylpropanediamine on Copper in Hot Water
H. Yoshioka, K. Yoshida, N. Noguchi, T. Ueki, K. Murai, K. Watanabe, M. Nakahara
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^{14}N NMR Evidence for Initial Production of NH_3 Accompanied by Alcohol from the Hydrolysis of Ethylamine and Butylamine in Supercritical Water
K. Yoshida, H. Yoshioka, N. Ushigusa, M. Nakahara
Chem. Lett., 50, 316-319, 2021

Dynamics and Chemical Reactions of Supercritical Water
M. Nakahara
Last Activity Report of the 183rd JSPS Committee on Advanced Water Science and Engineering, 18-19, 2021 (in Japanese)

Uchida, Hiroshi
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Sedimentary supply of humic-like fluorescent dissolved organic matter and its implication for chemoautotrophic microbial activity in the Izu-Ogasawara Trench
M. Shigemitsu, T. Yokokawa, H. Uchida, S. Kawagucci, A. Murata
Sci. Rep., 11, 19006 (10 pages), 2021

El Niño-Related Vertical Mixing Enhancement Under the Winter Mixed Layer at Western Subarctic North Pacific Station K2
A. Nagano, M. Wakita, T. Fujiki, H. Uchida
J. Geophys. Res. Oceans, 126, e2020JC016913 (18 pages), 2021

A Global Ocean Oxygen Database and Atlas for Assessing and Predicting Deoxygenation and Ocean Health in the Open and Coastal Ocean
M. Grégoire, V. Garçon, H. Garcia, D. Breitburg, K. Isensee, et al., H. Uchida, et al.
Front. Mar. Sci., 8, 724913 (29 pages), 2021

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Measurements and Modeling of the Vapor–Liquid Equilibrium Properties of Low-Global-Warming-Potential Refrigerant R32/R1234yf/R1123 Ternary Mixtures
H. Miyamoto, Y. Nakamura, K. Minai, T. Yamada
Fluid Phase Equilib., 558, 113440 (11 pages), 2022

Measurement of the vapour–liquid equilibrium properties of binary mixtures of the low-GWP refrigerants R1123 and R1234yf
H. Miyamoto, M. Nishida, T. Saito
J. Chem. Thermodyn., 158, 106456 (6 pages), 2021

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