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Ting Ruan

Jennifer Field

Ian Cousins

Rainer Lohmann

University of Rhode Island, rlohmann@uri.edu

Guibin Jiang

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Emerging Contaminants: Fluorinated Alternatives to Existing PFAS

Per- and polyfluoroalkyl substances (PFAS) are a class of anthropogenic chemicals that have extensive applications in industry and daily life. Once released into the environment, due to high stability of perfluoroalkyl moieties, PFAS are highly persistent and some are also bioaccumulative and toxic. Well-known legacy PFAS, particularly the long-chain perfluoroalkyl carboxylic acids (PFCAs) and perfluoroalkane sulfonic acids (PFSAs), have been subject to considerable public scrutiny, because of their ubiquitous presence in environmental compartments and biological species including human beings. Positive correlations between concentrations of long-chain PFCAs and PFSAs and multiple toxic/physiological indicators have been observed in laboratory exposure and epidemiology studies. Acid, salts, and related compounds of both the perfluorooctane sulfonate (PFOS) and perfluorooctanoate (PFOA) have been listed in Annexes of the Stockholm Convention for restricted use, and voluntary phase-out initiatives have been performed.

Nevertheless, it is not the end of story. An enduring environmental legacy of PFAS will remain long after their uses are discontinued. More importantly, a myriad of alternative PFAS with diverse molecular structures have emerged in the marketplace, with knowledge gaps on presence, transport and fate, as well as effects of these compounds. For instance, there are many thousands of PFAS listed in various databases (e.g., in the OECD Comprehensive Global Database) and research is underway to better understand the large PFAS universe.

Environmental Science & Technology (ES&T) is at the forefront of PFAS research since the first publication in the 1990s. Seminal scientific investigations published in *ES&T* have provided information on the composition, behavior, hazardous effects, treatment techniques, and management policies for PFAS, and continue to provide creative suggestions for the reduction and control of this group of environmentally persistent pollutants. A particular focus of this special issue are fluorinated alternatives to legacy PFAS with a collection of articles that provide important snapshots for a variety of emerging analogues.

This special issue coincided with “FLUOROS Global”, which was a combined in-person and virtual, regional event held October 3 – 7, 2021 at the WaterFire Arts Center in Providence, RI. FLUOROS Global 2021 addressed the rapidly evolving landscape of detection, health effects, regulation, remediation, and community response to PFAS contamination. National and international PFAS experts discussed state-of-the-art research and put forth their insights on advances in the field to the benefit of consumers, manufacturers, oversight and environmental agencies, and global health specialists. Participants included established and early career scientists, government officials (international, federal, state, and local), impacted community members, journalists, environmental NGOs, and PFAS-linked product manufacturers.

The special issue contains 23 papers, including 21 research papers, a feature article, and a critical review. Contents in the special issue cover a broad range of topics that include (1) methodology to characterize the structural diversity of PFAS alternatives; (2) environmental distribution, bioaccumulation, transfer, and ecological impacts; (3) transformation in the atmosphere and model animals; (4) human exposure, epidemiology, and toxicological impacts; (5) degradation and treatment techniques; and (6) strategy for PFAS control.

In this special issue, papers describe the significant progress made in understanding fluorinated alternatives. Current research tools, including target and nontarget analysis, oxidation and reduction, and endpoint evaluation, are effectively used to characterize chemical structure, evaluate environmental behaviors, and prioritize analogues with significant ecological impacts. Common characteristics are found between several kinds of fluorinated alternatives and legacy analogues in terms of bioaccumulation, distribution and transfer, and exposure routes. Moreover, creative trials in the aspects of biological effect evaluation, catalytic and adsorptive elimination, safety of fluorinated and PFAS-free alternatives, and implementation of the essential-use concept are emerging. The understanding of the degradability of certain molecular substructures (e.g., polyfluoroalkyl ether thiol alcohol, tertiary carbon unit, and chlorine substitution) might also provide feasible ideas for the design of less persistent and bioaccumulative analogues and for the reduction of existing fluorinated alternatives.

As guest editors of this special issue, we would like to thank all authors for the thoughtful views and excellent contributions. All reviewers are much appreciated for the active responses and constructive suggestions. A pivotal purpose of this special issue is to remind scholars with broad knowledge backgrounds that now is the time to express opinions and make contributions, so as to provide scientific and technical solutions for prioritization methods of analogues that are of high concern, comprehensive and reasonable toxicity assessment systems, more efficient treatment and reduction technologies, and sustainable regulatory policies.

Biographies

Ting Ruan is a professor at the State Key Laboratory of Environmental Chemistry and Ecotoxicology, Research Center for Eco-Environmental Sciences (RCEES), Chinese Academy of Sciences (CAS), China. He received a B.S. in environmental sciences in University of Science and Technology of China, and a Ph.D. from RCEES, CAS. Professor Ruan's research focuses on the development of analytical methodologies for the identification of novel organic pollutants in the environment.

Jennifer Field has a Ph.D. in geochemistry from the Colorado School of Mines. Her current research focuses on the development and application of quantitative analytical methods for organic micropollutants and their transformation products in natural and engineered systems with a focus on per- and polyfluoroalkyl substances (PFAS). Early in her career, she focused on field-based research to investigate the fate and transport of surfactants in groundwater and wastewater treatment systems. She is considered a pioneer in the area of PFAS occurrence and behavior and has focused on groundwater contaminated by fire-fighting foams and PFAS in municipal wastewater treatment systems and in municipal landfill. Current work focuses on the development of PFAS fingerprinting sources, characterizing PFAS in landfill gas, and PFAS on specialized textiles and other materials. She serves as an Executive Editor for *Environmental Science and Technology* and was an editor for *Water Research* from 2004-2008.

Ian Cousins is a Professor at the Department of Environmental Science, Stockholm University. He has a B.Sc. in Chemistry and a Ph.D. in Environmental Science. Prof. Cousins is well known for his research on the sources, transport and fate, and exposure pathways of PFAS. He is Associate Editor of the ACS journals *ES&T* and *Environmental Au*.

Rainer Lohmann is a Professor at the University of Rhode Island's Graduate School of Oceanography. He has a degree in Chemical Engineering and Doctorate in Environmental Science. He is Director of the URI-led Superfund Research Program Center on the Sources, Transport, Exposure and Effects of PFAS (STEEP). Prof. Lohmann has been member of *ES&T*'s Editorial Advisory Board since 2016. His research focuses on the detection, fate and transport of anthropogenic pollutants in the environment, often relying on passive samplers in the process.

Guibin Jiang is a professor at the Research Center for Eco-Environmental Sciences (RCEES), Chinese Academy of Sciences (CAS). He received a B.S. in analytical chemistry from Shandong University and an M.S. and Ph.D. in environmental chemistry from RCEES, CAS. Professor Jiang was invited to join the editorial advisory

board of *ES&T* in 2003 by the former Editor-in-Chief Prof. Jerald Schnoor. As the first Asia-based associate editor of *ES&T*, he has been appointed to direct the *ES&T* Asian Office since 2006. He is a recipient of the 2021 ACS Outstanding Achievements in Environmental Science & Technology Award. The main area of Prof. Jiang's research is focused on the identification, fate, exposure, and health effects of persistent and toxic substances. Other areas of interest involve chemical speciation analysis, analytical instrument innovation, environmental toxicology, impacts of nanomaterials, and isotope tracing techniques. Jiang has published over 1000 peer-reviewed papers, and is the author of more than 20 books.