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Editorial

Data Science for the Transformation of Environmental and Chemical Research and Development

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Environmental and chemical systems are complex in nature and often require major efforts in collecting, processing, and analyzing large data sets to uncover hidden patterns, correlations, and fundamental insights. Big data tools such as machine learning (ML) and artificial intelligence (AI) are transforming the ways of science discovery and technology development, and the journals *Environmental Science & Technology*, *Environmental Science & Technology Letters*, and *ACS Sustainable Chemistry & Engineering* have been at the forefront of publishing high-quality research on ML/AI in environmental and chemical fields.

In this joint virtual collection, we highlight 45 papers from these three journals that represent the breadth, depth, and influence of data science in environmental and chemical research. With ML/AI gaining tremendous momentum and with its wider adoption, these studies also demonstrate good examples of how to conduct "hypothesis-driven" research by using ML/AI tools to answer research questions and solve problems rather than descriptive and comparative work focusing on model comparisons.

This Virtual Issue is accompanied by the upcoming Special Issue on "Data Science for Advancing Environmental Science, Engineering, and Technology", and it is a follow-up on recent Global Webinars on data science topics "Bridging the Gap: Linking Analytical Chemistry to Biological Effects" and "ES&T: What was and what's next?" As we recognize and appreciate the power and value of ML and AI, we encourage you to submit the best work to the special issue.

These 45 articles selected from the three journals cover a wide spectrum of topics and shed light on the opportunities and best practice for advancing research using the emerging data science tools. Broadly, these topics cover analyzing and predicting chemical reaction and sorption behaviors, characterizing the distributions of contaminants throughout large areas, classifying and determining chemical activity and toxicity, estimating air quality at large spatial or temporal scales, designing and discovering new materials, multiobjective optimizations of systems and processes, and text mining for research topic exploration. The data sets are also diverse, ranging from big data collected from the literature, site monitoring, and lab research to citizen science projects.

Many common and novel ML/AI tools have been used in these studies. Popular supervised learning methods such as feedforward neutral networks, decision tree, and k-nearest neighbors (KNN) have been tested to seek desired outputs and outcomes, and unsupervised learning or reinforcement learning tools such as cluster analysis, principal component analysis (PCA), and self-organizing maps have been implemented to help with better prediction and decision making. Interestingly, several studies also used complementary experimental and machine learning approaches together to improve our understanding of chemical behaviors and to develop new tools for material screening and characterization.

The selected articles in this Virtual Issue are from more than 12 countries and regions around the world, and many studies were collaboratively performed by researchers from multiple regions. This reflects the global significance of the journals as well as the nature of ML/AI research in identifying, analyzing, and solving global environmental problems.

We believe data science tools will continue transforming the world and the way we live and work. This virtual collection is just a glimpse of how this got started. As we embrace a data-driven world together, we hope these articles inspire new research ideas and methods, foster new collaborations, and encourage your new submissions to the journals.

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Notes

Views expressed in this editorial are those of the authors and not necessarily the views of the ACS.

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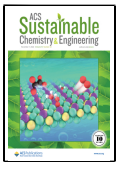

Biography

Zhiyong Jason Ren is a Professor in the Department of Civil and Environmental Engineering and the Andlinger Center for Energy and the Environment at Princeton University. His research focuses on the decarbonization and digitalization of environmental and chemical sectors. His group uses electrochemistry, microbiology, and data science tools to understand the fundamental determining factors and develop models and technologies for resource recovery during environmental and chemical processes. Prof. Ren is a Topic Editor of *Environmental Science & Technology* and *Environmental Science & Technology Letters*.

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