

# CSDS 500 and ECSE 500 Fall 2021 Colloquium

11:30AM to 12:30PM  
Thursday, October 21, 2021  
Hybrid: White 411 or Virtual

Zoom Webinar ID: 940 7438 8634  
Passcode: 357363

## “Machine Learning Modeling for the Reactivity of Contaminants in Engineered and Natural Environments”

**Abstract:** To mitigate and assess the risks associated with thousands of contaminants in engineered and natural environments, we need accurate predictive models that can readily provide reasonable estimates of their reactivity, both during important water treatment processes, including advanced oxidation processes (AOPs) and adsorption, and in the environment, such as through sorption on soils/sediments. However, conventional models rely heavily on quantitative structure-activity relationships (QSARs) between molecular descriptors and chemical activity which have multiple limitations, such as small numbers and narrow-scopes of contaminants involved, tedious calculations of molecular descriptors, and ignorance of adsorbent properties. In this talk, we'll discuss our recent progresses in using machine learning algorithms to develop more powerful, robust, and trustworthy predictive models. Specifically, we have 1) mined the literature and available databases to obtain large datasets of contaminant reactivity in AOPs and adsorption; 2) experimentally quantified the activity of selected contaminants in AOPs or adsorption; 3) developed predictive machine learning models for the activity of contaminants based on the data from the above two objectives; and 4) interpreted the obtained machine learning models to make them trustable and defined their applicability domains.



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**Bio:** Dr. Huichun (Judy) Zhang is the Frank H. Neff professor in the Department of Civil and Environmental Engineering at Case Western Reserve University. She earned her Ph.D. from Georgia Institute of Technology and her B.S. and M.S. from Nanjing University in China. Her research focuses on the fate and transformation of environmental contaminants in natural and engineered aquatic environments and the removal of organic contaminants from contaminated water. Her recent research areas also include predictive modeling for contaminant reactivity and sorption using both classical models and machine learning tools. Dr. Zhang has published in numerous journals, such as Chemical Reviews, Environmental Science and Technology, Water Research, Chemical Engineering Journal, Journal of Physical Chemistry C, Langmuir, Applied Catalysis B, Journal of Agriculture and Food Chemistry, Chemosphere, and Journal of Hazardous Materials. She has received six competitive research grants from the U.S. National Science Foundation as the PI. In addition, Dr. Zhang directed research projects for USDA, US EPA, OWDA, PennDOT, William Penn Foundation, NSF WET Center, USGS through PA-WRRC and PA Sea Grant, and Research Corporation. She is an Associate Editor for Environmental Research, Frontiers of Environmental Science and Engineering (FESE), and Journal of Environmental Engineering (ASCE).

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