Tuning gas interactions at solid-water interfaces from the Angstrom-to-field scales for sustainable gas transport, recovery, and storage in extreme environments

Abstract: Connecting the sub-nano- and meso-scale interactions of gases with hierarchical and heterogeneous materials in natural and engineered processes has applications for many areas such as the geologic storage of CO$_2$, enhanced hydrocarbon recovery, noble gases as tracers for hydrocarbon or CO$_2$ migration, and limiting the diffusion of H$_2$ from the corrosion of radioactive waste containers to prevent explosions. Other critical technical challenges in sustainable energy and environment are the development of thermodynamically downhill routes for CO$_2$ conversion and the safe and permanent storage of CO$_2$. To address these technical challenges, the diffusivity and partitioning behavior of the gases in confined pore spaces are determined using molecular dynamics simulations. These studies are complimented by in-operando multi-scale X-ray and neutron scattering measurements (USAXS/SAXS/WAXS and USANS/SANS) of gas interactions with hierarchical materials such as clays at elevated temperatures and pressures ($T_{\text{max}}$ = 90°C, $P_{\text{max}}$ = 80 bar). Further, the engineered conversion of CO$_2$ to carbonates in heterogeneous materials (e.g., Ca- and Mg-silicates minerals and rocks), and the tuning of carbonate morphology and structure for integration with the built environment are investigated. The implications of these results for engineering complex interfaces for sustainable energy and resource recovery are evaluated.

Biography: Dr. Greeshma Gadikota is an Assistant Professor in the Department of Civil and Environmental Engineering with appointments in the Environmental Chemistry and Technology Program, Geological Engineering Program, and the Wisconsin Energy Institute. She runs the Sustainable Energy and Resource Recovery Group at UW-Madison. Previously, she was a postdoctoral research associate in the Department of Civil and Environmental Engineering at Princeton University, and a research associate in the Materials Measurement Science Division at the National Institute for Standards and Technology (NIST). Dr. Gadikota was selected as the Rising Stars in Civil and Environmental Engineering by MIT in 2015. She served as the technical coordinator for the Research Coordination Network in Carbon Capture, Utilization, and Storage (RCN-CCUS) supported by the National Science Foundation. Dr. Gadikota received her PhD in Chemical Engineering from Columbia University in 2014. She earned her MS degrees in Chemical Engineering (2011) and Operations Research (2008) also from Columbia University and her BS in Chemical Engineering (2007) from Michigan State University. Her research interests are aimed at integrating in-operando and in-silico characterization of complex hierarchical and heterogeneous materials with multi-scale reaction kinetics and gas transport mechanisms. Her research connects sub-nano- to meso-scale measurements with process-scale developments and field-scale observations, using advanced synchrotron characterization methods, molecular dynamics simulations, and laboratory scale measurements. The key application areas of this approach include carbon capture, utilization, and storage, enhanced gas recovery, nuclear waste storage, and the production of high-value materials from low-value substrates.

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