Advances and new challenges in molecular-scale interfacial reactions and applications to sustainable remediation of contaminants

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The study of interfacial reactions at the molecular scale that control the speciation, mobility, and transformation of environmental contaminants has expanded greatly over the last 30 years. Significant advances in fundamental knowledge can be attributed to the development and increased accessibility of a variety of spectroscopic and microscopic methods together with developments in theoretical and computational chemistry. Our ability to interrogate, observe, and model molecular-scale environmental reactions has reached unprecedented levels. Concurrently in the last decade, sustainable approaches for the remediation of contaminants in water, soil, and sediments have been widely embraced and promoted by government and industry alike. Monitoring and remediation technologies, methods, and practices are sought that are both cost-effective and offer resiliency towards unpredictable impacts of climate change. In what ways can research at the molecular scale contribute to new knowledge of contaminant transformation and fate, as well as to sustainable and resilient remediation? The need for chemistry-based mechanistic understanding in the context of remediation is most critical for contaminants at low concentrations, in environments with poor accessibility, and that exhibit complex behavior; i.e., contaminants that readily and rapidly change oxidation state, chemical form, molecular size, or bioavailability in response to local biogeochemical conditions. This talk will review advances, new challenges, and research opportunities related to molecular-scale reactions and sustainable remediation in two areas: (i) application of coupled thermodynamic, kinetic, and transport models as an integrator, simulator, and forecaster of multi-variant complex systems involving contaminants; and (ii) mechanism-based design of novel remediation technologies using reactive soil or sediment amendments.