Molecular Level Design of High-Performance Sorbents

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A combination of quantum mechanical calculations, large-scale molecular dynamics, and surface complexation modeling have been used to study how contaminant ions sorb to the surfaces of inorganic oxides. Insights from these studies have been used to design and synthesize new materials that effectively and inexpensively remove contaminant ions from aqueous solutions. The application of these materials to nuclear waste sequestration, environmental remediation and drinking water treatment will be discussed.