# Research Highlights of Atomistic Modeling and Simulation Group

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Our research aims to garner better understanding of complex physicochemical processes in nature, such as phase transitions, melting of nano-clusters, solvation, H-bonding, reaction mechanisms, swelling of clay-minerals, proton transport, fast ion transport in solids, etc. We employ variety of atomistic computer simulation techniques, such as classical and *ab-initio* molecular dynamics (MD), Monte Carlo (MC), metadynamics (MTD), etc. in this pursuit. Currently, we are specifically focusing on the following two areas,

1. **Fast-ion transport in solids:** The phenomenon of *superionic* conductivity in solids is technologically very important for the development of next generation high-energy-density portable energy devices, such as batteries and fuel cells. Employing variety of state-of-the-art computational tools, we explore factors that govern ion mobility in variety of solid solutions, that are high conducting due $Li^+$ or $Na^+$, for potential applications as solid electrolytes in rechargeable batteries. These studies are currently extended to proton ($H^+$) and oxide-ion ($O^{2-}$) ion conducting solids for applications in solid oxide fuel cell (SOFC) devices.
2. **Water remediation and Corbon sequestration:** Surveys across different regions of the globe suggest surging levels of harmful pollutants, such as of arsenic and selenium, in ground-water as well as in rivers. Water remediation through confinement of these toxic water-borne species is extremely important for environment conservation, and sustenance of life on Earth. So are the concerns over the green-house gases, such as $CO_2$ and $CH_4$. We examine the nature of solvation and speciation of toxic poly-atomic species, such as $SeO^{3-}$, $HSeO^{4-}$, $H_2AsO_3^-$, $HAsO_3^{2-}$, etc., in water to help the development of water remediation strategies. Currently we are extending this study for carbon ($CO_2$) sequestration using alkali carbonates solutions.

In these computational studies, we extensively use freely available software tools for data generation. However, development of indigenous data analysis tools need be developed to garner fresh insights that are meaningful for scientific advancements.

*Note:* Students interested in these computational topic should have good understanding of classical mechanics and statistical physics, in addition to aptitude for computer programming.

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