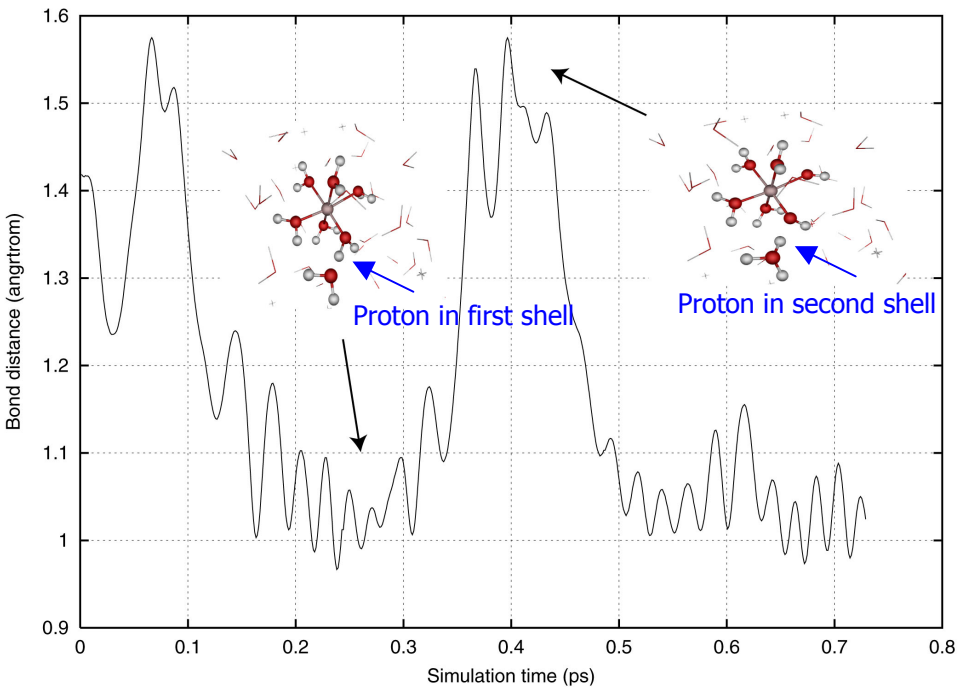
GC-8 Highlight

UCSD, EMSL

Ab Initio Molecular Dynamic (AIMD) Simulations of Proton Exchange Around Highly Charged Ions in Solution



The properties of ions in aqueous solutions is of enormous importance to the interpretation of processes as diverse as biological function of proteins, subsurface transport, mineral formation, and the cleanup of toxic waste. In these systems the interaction of the ion with the surrounding water molecules leads to strong polarization which impacts all aspects of aqueous complexation. The figure illustrates proton motion seen in an ab initio MD simulation of the hydrolysis of the Al^{3+} ion. Very small barriers are seen for proton transfer from the first solvation shell to the second solvation shell. Ab initio MD simulations can provide critical insight into these types of speciation effects as well as for oxidation reduction reactions which require understanding the coupling of proton transport and electron transport.

M.I. Lubin, E. J. Bylaska, J.H. Weare (2000), Chem. Phys. Lett., 322, pp. 447-453

M. Valiev, E. J. Bylaska, A. Gramada, J.H. Weare, in Reviews in Modern Quanum Chemistry: A Celebration of the Contributions of R.G. Parr Ed. K.D. Sen (World Scientific, Singapore) in press.

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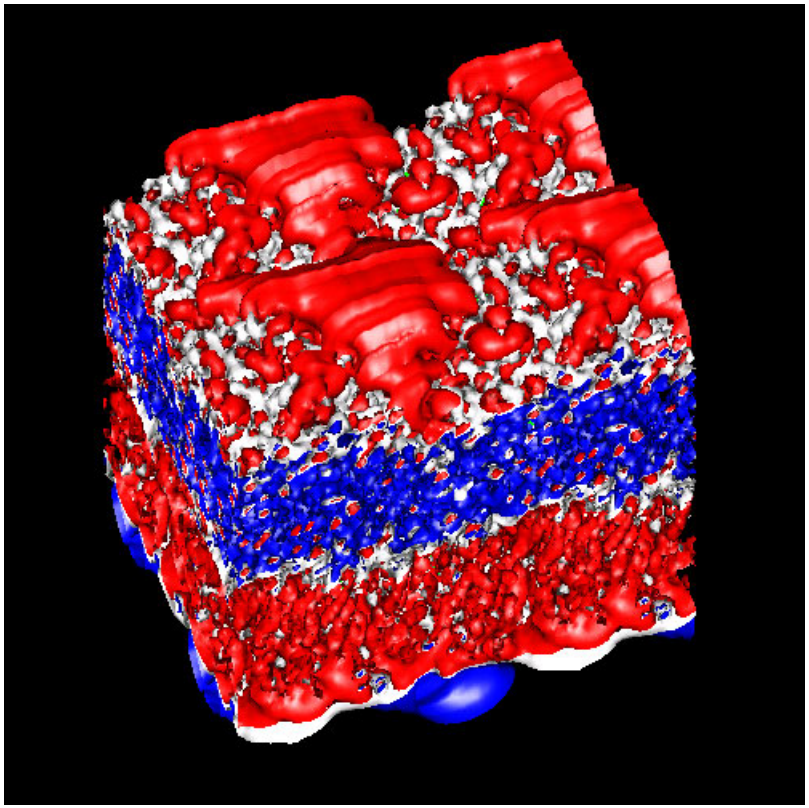
GC-8 Highlight

EMSL

Geochemical Reactions at Microbial Membranes



Certain species of Gram-negative bacteria are able to take up and reduce metal ions from their environment. This ability, as well as the adhesion of these microbes to mineral surfaces has been shown to be mediated by the lipopolysaccharide (LPS) molecules that form the main constituent of the outer bacterial membrane. Understanding the detailed molecular interactions at the microbial surface is essential for the design of new remediation strategies. A new approach to evaluate the electrostatic potentials from *ab inito* electronic structure calculations was used to determine partial atomic charges of the 936-atom LPS molecule of *Salmonella typhimurium*, and the 474-atom LPS molecule of *Pseudomonas aeruginosa*. Classical molecular dynamics simulations provided trajectories for the first dynamic electrostatic potential analysis of the LPS/phospholipid bilayer membrane of *Pseudomonas aeruginosa*. The simulations provide new insight in the ion transport and adhesion properties of microbial membranes.

R. D. Lins and T. P. Straatsma, Computer simulations of the lipopolysaccharide membrane of *Pseudomonas aeruginosa*. *Biophysical Journal*, **81**, 1037-1046 (2001).

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