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Molecular dynamics investigation of surface potential and electro-kinetic phenomena at the amorphous silica/water interface

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The static and electro-kinetic properties of amorphous silica-aqueous electrolyte interface are of long-standing scientific interest and current technological relevance. Different theoretical models of the electrical double layer (EDL) have been used to explain a wide range of experimental measurements, including zeta potential, second harmonic generation (SHG), sum frequency generation (SFG), electro osmotic flow (EOF), and streaming potential. Using extensive molecular dynamics simulations, we have studied this EDL as a function of salt concentration for a silica surface charge density of -0.82e/nm^2 (e=electron charge). The simulation results can be captured with a simple model by breaking the double layer region into three zones: an inner region in which the Na^+ counter-ion population is independent of [NaCl] and there are no Cl^- co-ions, an intermediate region which hosts a population of non- exchangeable Na^+ plus another group of Na^+ and Cl^- ions whose population is described by a Langmuir adsorption model, and an outer region where the ion distribution is well-described using Poisson-Boltzmann theory. To compare the applicability of our and other EDL models, e.g. the Gouy-Chapman, the constant-capacitance, and the triple-layer models, we analyze experimental data of SHG and streaming potential. We investigated the implications for interpretations of the results using different models, and scrutinize the correctness of the underlying physics.

Biography

Si-Han Chen has completed his PhD at the age of 32 years from the Ohio State University and he is now a postdoctoral researcher from the University of California, Riverside. He has published more than 7 peer-reviewed papers in experimental and theoretical chemistry. His current research field is binding kinetics of enzyme using machine learning-based methods.

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