Hydrogen bonding and ultrafast dynamics at aqueous-oxide interfaces

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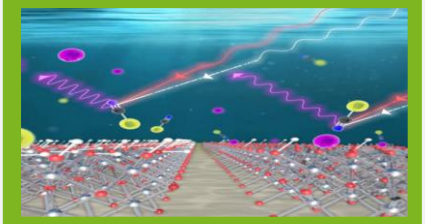
Chemistry Seminar on the *Interfacial dynamics*



Monday Feb. 12 at 4 pm in 303 Schrenk

Please contact Dr. Garry Grubbs at grubbsg@mst.edu for further information.

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Abstract: Interfacial water structure is key to diverse chemical and physical processes, including many of environmental and geochemical relevance. It can be probed by vibrational sum-frequency generation (vSFG) spectroscopy as well as ultrafast time-resolved vSFG. Combined with computational tools, such as molecular dynamics simulations, a microscopic understanding of interfaces can be approached. Our experiments show that in the absence of surface charge (pH 2), water at silica surfaces exhibits significantly slower OH stretch vibrational relaxation (~600 fs) compared to bulk water. However, at charged silica surfaces (e.g., pH 6), bulk-like fast dynamics (~200 fs) are observed at low ionic strength. This decelerates to ~600 fs with the addition of NaCl. In parallel, vSFG results demonstrated that silica interfacial water structure is most sensitive to ions at pH=6-8, correlating with the known salt and pH dependence of silica surface reactivity. Consequently, it is unclear whether the observed slowing of the vibrational dynamics is due to the reduction in the Debye length, or because of changes in the local hydrogen bonding environment caused by the electrolyte and how this might depend on the identity of the ions or the solid surface. The combination of molecular dynamics simulations with spectroscopic and time-resolved vSFG experiments on aqueous Al_2O_3 interfaces, along with the use of a molecular probe (SCN^-), sheds light on the ongoing debate on the role of ions in interfacial water structure and the hydrogen bonding network, as well as whether the observed behavior is specific to silica/water interfaces or can be generalized to other aqueous interfaces.

About the speaker: Dr. Eric Borguet is the inaugural Hazel Tomlinson Professor of Chemistry at Temple University in Philadelphia, PA. He was born in Dublin, Ireland, where he spent his formative years. He attended college in France at the Université de Paris-Sud (XI-Orsay) where he studied chemistry and physics. He traveled to Philadelphia, Pennsylvania in the USA and obtained his Ph.D. in Physical Chemistry at the University of Pennsylvania in 1993, under the mentorship of Professor Hai-Lung Dai where he investigated adsorption and intermolecular interaction on stepped metal surfaces. His post-doctoral training was completed at Columbia University in the group of Professor Kenneth Eisenthal using nonlinear optics to investigate spectroscopy and ultrafast dynamics at liquid interfaces.

Chemical and physical processes at surfaces and interfaces are the principal focus of his ongoing research program at Temple University. His research activities have resulted in over 150 peer-reviewed publications, in excess of 300 invited talks and more than 280 contributed presentations. in excess of 300 invited talks and more than 270 contributed presentations.