

Fritz-Haber-Institut der Max-Planck-Gesellschaft

Physikalische Chemie — Direktor: Prof. Dr. Martin Wolf



MAX-PLANCK-GESellschaft

Department Seminar:

Wednesday, January 23, 2019, at 11:00 a.m.;

— all are invited to meet at around 10:40 for a chat and coffee —

Prof. Dr. Eric Borguet

Department of Chemistry,
Temple University, Philadelphia PA.

The impact of ions on ultrafast vibrational spectroscopy and dynamics at aqueous interfaces

PC Seminar Room G2.06, Building G

K. Campen

Abstract:

Interfacial water structure is key to many chemical and physical processes. It can be probed by vibrational sum-frequency generation (vSFG) spectroscopy as well as ultrafast time-resolved vSFG. However, a more complete microscopic understanding requires additional techniques such as molecular dynamics simulations. 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 Al₂O₃ interfaces sheds light on the ongoing debate on the role of ions in interfacial water structure and whether the observed behavior is specific to silica/water interfaces or can be generalized to other aqueous interfaces.