

Effect of H₂SO₄ and Alkali Metal SO₄²⁻/HSO₄⁻ Salt Solutions on Surface Water Molecules Using Sum Frequency Generation

Steve Baldelli, Cheryl Schnitzer, and Mary Shultz

Department of Chemistry, Tufts University, Medford, Massachusetts 02155

D.J. Campbell

Department of chemistry, College of the Holy Cross, Worcester, Massachusetts 01610

Journal of Physical Chemistry **103**, 2789 - 2795, 1999.

The surface-specific vibrational spectroscopy, sum frequency generation, has been used to study the structure of water at air/liquid interfaces of inorganic, ionic solutions. The experiments suggest that ions in solution reorient surface water into a more structured, hydrogen-bonded network compared with the neat water/air interface. In more concentrated solutions, there is a high degree of ion association. A model based on Hard Soft Acid Base theory indicates that associated ions are able to penetrate closer to the air interface than unassociated ions. Associated ions incorporate surface water into the ion-pair hydration shell.