Characterizing Water Cluster Anions by Quantum Simulation

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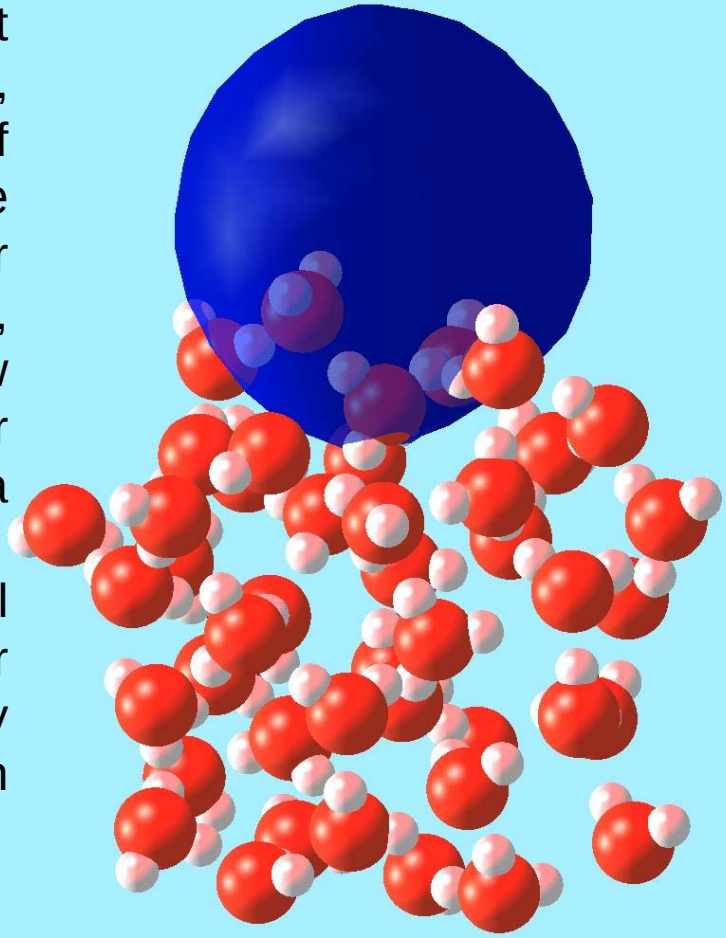
Molecular clusters are not only of direct chemical importance, e.g., in the atmosphere, but can also act as a window for observation of the chemical processes that occur in the more complex environment of liquid solutions. For negatively charged water clusters, however, experiment has been unable to determine how the excess electron is bound to the molecular assembly, as an interior, bulk-like, state or as a surface associated electronic state.

Simulations yield energetic and spectral data which show that the trends with cluster size observed in experiment are reproduced by a sequence of surface states, not accessible in a bulk liquid, up to quite large cluster size.



L. Turi, W-S. Sheu, and P.J. Rossky, "Characterization of Excess Electronic States in Water Cluster Anions via Quantum Simulations." Science 309, 914-917 (2005).