Hydrated Proton Clusters

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A potential energy surface for $(H_2O)_nH^+$ has been developed based on extensive *ab initio* calculations for $H_5O_2^+, H_3O^+, H_9O_4^+$, and $(H_2O)_2$ It has been tested in simulations of pure water clusters, bulk water, and these same systems containing an excess proton. Features of the potential energy surface are explored in this presentation. An analysis of the radical structural changes that accompany addition of an excess proton to a water cluster is presented. Preliminary results of vibrational calculations in these systems is presented.