

Abstract Submitted
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Dielectron Attachment and Hydrogen Evolution Reaction in Water Clusters¹ ROBERT BARNETT, Georgia Institute of Technology, RINA GINIGER, ORI CHESHNOVSKY, Tel-Aviv University, UZI LANDMAN, Georgia Institute of Technology — Binding of excess electrons to nano-size water droplets, with a focus on the hitherto largely unexplored properties of doubly-charged clusters, were investigated experimentally using mass spectrometry and theoretically with large-scale first-principles quantum simulations. Doubly-charged clusters were measured in the range of $83 \leq n \leq 123$, with $(\text{H}_2\text{O})_n^{-2}$ clusters found for $83 \leq n < 105$, and mass-shifted peaks corresponding to $(\text{H}_2\text{O})_{n-2}(\text{OH}^-)_2$ detected for $n \geq 105$. Simulations revealed surface and internal dielectron, e_2^- , localization modes and elucidated the mechanism of the reaction $(\text{H}_2\text{O})_n^{-2} \rightarrow (\text{H}_2\text{O})_{n-2}(\text{OH}^-)_2 + \text{H}_2$ (for $n \geq 105$), which was found to occur via concerted approach of a pair of protons belonging to two water molecules located in the first shell of the dielectron internal hydration cavity, culminating in hydrogen formation $2\text{H}^+ + e_2^- \rightarrow \text{H}_2$. Instability of the dielectron internal localization impedes the reaction for smaller ($n < 105$) clusters.

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