

Institutsseminar

Ionic Water Clusters: Magic Numbers, Hydrogen Scrambling

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Water cluster ions are fascinating subjects of study with a number of interesting properties; this presentation aim to cover two of them, namely, the so-called magic numbers and intra-cluster proton mobility.

Magic number clusters refer to the observation—first reported by Sin-Shong Lin in 1973—that in a mass spectrum showing a distribution of cluster sizes, some of them will be much more abundant than expected. In particular, the cluster comprising 21 water molecules and a proton has been the subject of many scientific works, both theoretical and experimental, over the years; here will be presented a work elucidating the structure of the cluster.

The proton mobility inside a water cluster ion is greatly dependent upon the type of core ion used as a charge carrier. This property can be probed by measuring the degree of hydrogen scrambling taking place in the cluster, *i.e.*, the degree to which the positions of the hydrogen atoms are randomized with regards to which oxygen atoms they are bound to. Examples are presented for a number of different core ions, such as, H_3O^+ , NH_4^+ , pyridinium and bisulphate.

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15:30 Uhr

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