SPECTRAL EVIDENCE FOR SURFACE BOUND ELECTRONS IN THE DOMINANT ISOMER OF LARGE WATER CLUSTER ANIONS

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Negatively charged water clusters are promising model systems for elucidating molecular level aspects of the hydrated electron. For the past twenty years the debate has centered on whether the excess electron is bound internally or on the surface in the readily available clusters (less than 100 water molecules). In these sized clusters, multiple isomer classes are known to exist. Clusters within each isomer class are thought to exhibit the same electron binding motif due to the smooth and continuous evolution of electron binding energy with increasing size. Recent studies of the ultra-fast relaxation dynamics of the larger sized clusters (50 - 100) have been interpreted in the context of an internally solvated excess electron for the dominant isomer class while the weaker binding class adopts a surface bound morphology. Studies of the dominant isomer in smaller water clusters indicate, however, that the electron is bound primary by one water molecule in a surface state. We have recently extended these studies of the dominant isomer class in both the water bending and stretching regions to include clusters of up to twenty water molecules. Surprisingly, the local electron binding motif persists even into the larger water clusters, suggesting a continuous electron accommodation morphology with increasing cluster size.