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Single and Double Excess Electrons in Water Clusters[1] YING LI, ROBERT BARNETT, UZI LANDMAN, School of Physics, Georgia Institute of Technology — Excess electrons in polar solvents is a topic of continuing interest. Early theoretical research on this subject predicted formation of surface and internal hydrated electron states, depending on the size of the water cluster and the state of the cluster [1]. Evidence for these modes of electron hydration has been reported in recent experiments. We discuss here theoretical investigations of excess electrons states in water clusters as a function of cluster size and state (liquid and frozen) using hybrid quantum (DFT)/classical simulations. In addition we discuss dielectron hydration in clusters [2]. [1] R. N. Barnett, C. L. Cleveland, U. Landman, J. Jortner, J. Chem. Phys. 88, 4429 (1988). [2] H.-P. Kaukonen, R. N. Barnett, U. Landman, J. Chem. Phys. 97, 1365 (1992).

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