Photoemission into water adsorbed on metals: probing dissociative electron transfer using theory

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Abstract

The photoinduced dissociation of water adsorbed on a silver nanoparticle is explored using theory to probe reaction pathways. Electron attachment of a photoemitted electron to adsorbed water can lead to the formation of H_2 at a very low energy barrier with oxygen remaining on the Ag surface. Another pathway releases a H atom, leaving OH on the surface. The transport of the released H atom to a nearby nanoparticle is also discussed. Results are also reported for electron transfer to a solvated lithium ion, $Li(H_2O)_6^+$, near the surface of a silver particle. *Ab initio* configuration theory is used to describe the systems and a formulation that allows excited electronic states embedded in a near continuum of lower energy states to be calculated accurately is discussed. Effects due to doping of a Ag nanoparticle with a K electron donor atom are compared with those caused by a Fermi level shift due to an applied potential.