Generation of hydrated electrons with visible light

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The hydrated electron is a metastable defect in liquid water which also exhibits an exceptional reactivity. While the hydrated electron is capable of reducing CO2 and N2 to CO and NH3, respectively, its current generation requires high energy photons. This can be overcome by using the heptazinyl radical (HzH) as a source of electrons. HzH is generated as an intermediate product in the water-splitting cycle catalyzed by heptazine (Hz). Combining the water-splitting reaction with the generation of hydrated electrons yields a photocatalytic reaction-cycle in which the Hz molecule is regenerated upon the formation of the hydrated electron.

Ab initio methods are employed to explore possible minimum-energy excited-state reaction paths for proton-coupled electron transfer from HzH to water. The results suggest a barrierfree exothermic reaction-pathway without conical intersections for the formation of hydrated electrons by photodetachment from the HzH radical.