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The Role of Hole Localization in Sacrificial Hydrogen Production by Semiconductor-Metal Heterostructured Nanocrystals[1] SCOTT LAMBRIGHT, KRISHNA P. ACHARYA, RONY S. KHNAYZER, TIMOTHY O'CONNOR, GEOFFREY DIEDERICH, MARIA KIRSANOVA, ANNA KLINKOVA, DANIEL ROTH, ERICH KINDER, MARTENE IMBODEN, MIKHAIL ZAMKOV — The effect of hole localization on photocatalytic activity of Pt-tipped semiconductor nanocrystals is investigated. By tuning the energy balance at the semiconductor-ligand interface, we demonstrate that hydrogen production on Pt sites is efficient only when electron-donating molecules are used for stabilizing semiconductor surfaces. These surfactants play an important role in enabling an efficient and stable reduction of water by heterostructured nanocrystals as they fill vacancies in the valence band of the semiconductor domain, preventing its degradation. In particular, we show that the energy of oxidizing holes can be efficiently transferred to a ligand molecule, leaving the semiconductor domain intact. This allows re-using the inorganic portion of the "degraded" nanocrystal-ligand system simply by recharging these nanoparticles with fresh ligands.

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Scott Lambright

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