Chlorine-passivated CdSe nanocrystal quantum dots: surface property relationship in photocatalytic hydrogen evolution.

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We demonstrate the role of chlorine (Cl) on the surface of CdSe nanocrystals (NCs) (Cl:CdSe NCs) in photocatalytic hydrogen evolution from water. Transient absorption spectroscopy implies that Cl helps remove electron trap states in CdSe NCs, resulting in an increase of photoluminescence quantum yield, e.g., from 9% to 21% after Cl treatment. Photocatalytic hydrogen evolution from water corroborates the effect of the surface Cl. In the case of large NCs, Cl:CdSe NCs show a high hydrogen-evolution rate, due to the passivation of trap states with energy levels below the reduction potential necessary for H2O reduction, while bare CdSe NCs exhibit slower reduction. In contrast, trap states do not come into play in the case of NCs less than 2.7 nm diameter as both the conduction band-edge and trap states are above the water reduction potential. Cl passivation resulting in a low concentration of trap states lowers the photocatalytic activity of water splitting, which is likely a result of impeded charge separation because of the absence of trap states.