The effect of chlorine passivation on photocatalytic hydrogen generation from CdSe nanocrystals

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In this work, we examine the photocatalytic H_2O splitting activity of chlorine passivated CdSe(Cl-CdSe) nanocrystals(NCs) depended on size of NC. It turned out that passivated chlorine diminish the trap state by removal of dangling bond on surface of CdSe NCs throughout the study of transient absorption spectroscopy. The photocatalytic activities of varying size of bare CdSe and Cl-CdSe are obviously contrasted. In the case of large size, Cl-CdSe NCs are shown to be strongly active for photocatalytic H_2 evolution, which is attributed to passivation of trap states with energies lying below the reduction potential necessary for H_2O reduction, while bare CdSe NCs reveal the weak activity due to the trap state. The other way, in the case of small size, trap state did not come into play for activity reduction by risen conduction band, is located above the H_2O reduction potential, due to the quantum confinement effect. Furthermore, absence of trap state by Cl treatment inhibits the charge separation, which was directly related to photocatalytic activity. Therefore, Cl-CdSe NCs show the weaker activity than bare CdSe in the contrast with case of large size. Thus, Cl treatment can manipulate surface trapping dynamics to dictate the photocatalytic activity.