Supporting Information

Photocatalytic H₂ production by a hybrid assembly of [FeFe]-hydrogenase model and CdSe quantum dot linked through a thiolato-functionalized cyclodextrin†

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**Fig. S1** UV-vis spectra of (a) β-CD-6-S-CdSe QDs sampled at the refluxing interval of 30 min and (b) MAA-CdSe QDs sampled at the refluxing interval of 3 h.
Fig. S2 Fluorescence spectra of (a) β-CD-6-S-CdSe QDs sampled at the refluxing interval of 30 min and (b) MAA-CdSe QDs sampled at the refluxing interval of 3 h.
Fig. S3 Mass spectrum of 1/β-CD-6-SH formed in situ in water.
Fig. S4 Cyclic voltammograms of β-CD-6-S-CdSe and MAA-CdSe QDs in water using a saturated KCl Ag/AgCl reference electrode at pH 4.5.
Fig. S5 Changes of UV-vis absorptions of β-CD-6-S-CdSe QDs in water at varying pH from 7 to 1.4.
**Fig. S6** Long-time photocatalytic H₂ evolution of the system of β-CD-6-S-CdSe QDs (1.0 × 10⁻⁴ M), 1 (1.0 × 10⁻⁵ M), and H₂A (0.28 M) in water at pH 4.5 under illumination, with addition of extra 1 or β-CD-6-S-CdSe QDs after 14 h of illumination.