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Surface Step Decoration of Isolated Atom as Electron Pumping: Atomic-Level Insights into Visible-Light Hydrogen Evolution

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Abstract

Here we realize the decoration of isolated platinum atoms onto the surface step of CdS nanowires. The single-atom co-catalyst with high stability can realize maximum atom efficiency and significantly boost electron-hole separation efficiency in chromophore units, generating a greatly enhanced photocatalytic hydrogen evolution performance, 7.69 times as high as Pt nanoparticles do and 63.77 times higher than that of bare CdS nanowires. Directional migrations of photogenerated excitons from the conduction band of CdS to catalytic platinum centers have been witnessed by transient absorption spectroscopy, leading to the supply of long-lived electrons for highly efficient photocatalytic hydrogen evolution. Density functional theory calculations further confirm that the excellent catalytic performance is associated with positively charged platinum sites with partially vacant 5d orbitals, which change distribution of charge density and facilitate higher excited carrier density.

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