Supporting Information

In Situ Growth of P-type CuSCN/Cu₂O Heterojunction to Enhance

Charge Transport and Suppress Charge Recombination

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The band gap calculation of CuSCN

The $(\alpha h\nu)^2$ vs photo energy plots are shown in **Fig. S1**, which is originated from the UV-visible spectra. The absorption coefficient α and optical band gap of the films were calculated by applying the Tauc model as follows^[1-3]:

$$\alpha = -\frac{1}{d}\ln(\frac{T}{1-R}) \tag{1}$$

$$\alpha h \nu = C (h \nu - E_g)^{1/2} \tag{2}$$

Where *T* and *R* are the transmittance and reflectance of films, *d* is the film thickness, *hv* is the photon energy, E_g is the optical bandgap, and *C* is the constant. E_g can be calculated by plotting $(\alpha hv)^2$ vs *hv* and by extrapolating the linear portion of the absorption edge to find the intercept with energy axis. The calculated optical band gap of CuSCN is 3.91 eV, which is higher than previous report (3.8 eV).^[4] This phenomenon may be attributed to the quantum size effect resulting from the nano-structure.^[5]

Research on different strong alkali treatment time

The structural morphology and charge transport performance of the CuSCN/Cu₂O can be adjusted by changing the treatment time of the strong alkali. The SEM patterns of CuSCN immersed in 0.1M NaOH aqueous solution for different times are shown in **Fig. S2**. It is found that, with the increase of the treatment time of strong alkali, the surface morphology is changed gradually from the initial nanorod to nanoneedle/ nanorod heterojunction structure. Besides, more and more nanoneedles are formed on the surface with the increase of treatment time. This confirms that the CuSCN/Cu₂O heterojunction structure can be achieved by simple alkali treatment. However, when the treatment time is over 90 s, the nanoneedle/nanorod heterojunction structure evolves gradually to nanorod. This may be attributed to that superabundant CuSCN is converted into Cu₂O.

The chopping photocurrent density of CuSCN (shown in **Fig. S3**) increases firstly and then decreases with the increase of treatment time. In the beginning, the formed CuSCN/Cu₂O heterojunction can promote charge transport and suppress charge recombination, thereby improving the chopping photocurrent density. But the chopping photocurrent density declines sharply when the treatment time is over 90 s. This may be resulted from poor conductivity of Cu₂O, which is consistent with SEM results.

In short, the photoelectric performance of CuSCN/Cu₂O heterojunction can be modified by alkali treatment time according to the different requirements. This will further expand the range of potential applications.



Fig. S1 The $(\alpha h\nu)^2$ *vs* photo energy plots of CuSCN.



Fig. S2 A-F represent the SEM patterns of CuSCN immersed in 0.1M NaOH aqueous solution for 0 s, 10 s, 30 s, 90 s, 180 s, 300 s, respectively.



Fig. S3 The chopping photocurrent density of CuSCN immersed in 0.1M NaOH aqueous solution for different times measured at 0 V vs. SCE under the irradiation of UV-365 ultraviolet lamp.

References

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