

## Electronic supplementary information (ESI)

### Two-dimensional layered CdS/C<sub>2</sub>N heterostructure for

### Visible-Light-Driven Photocatalysis

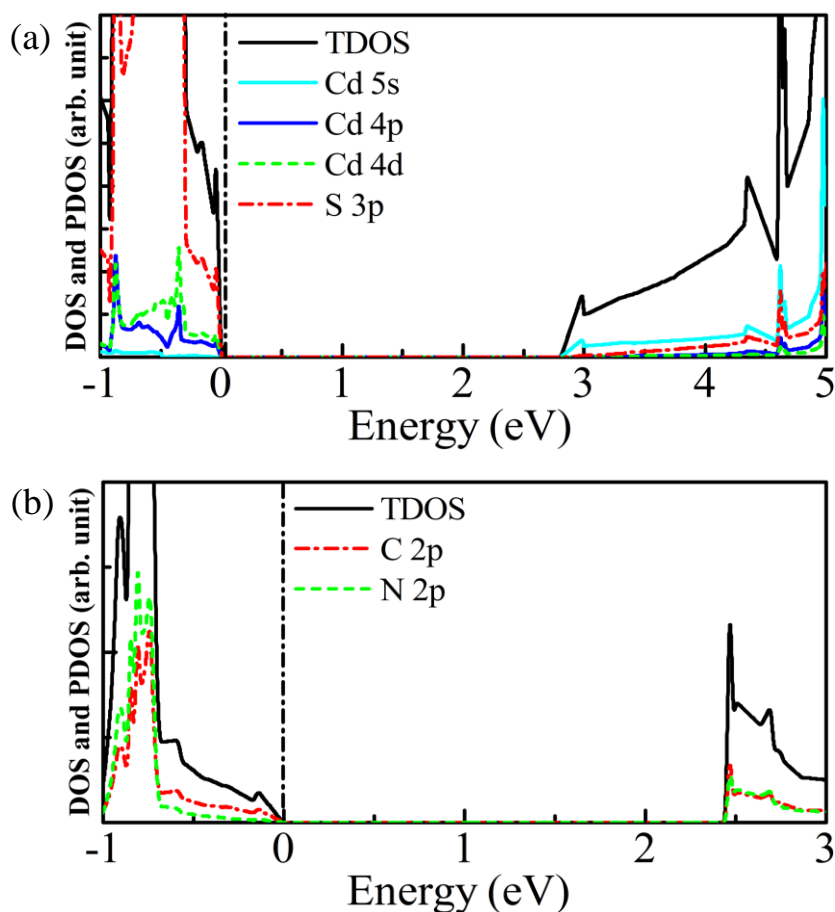
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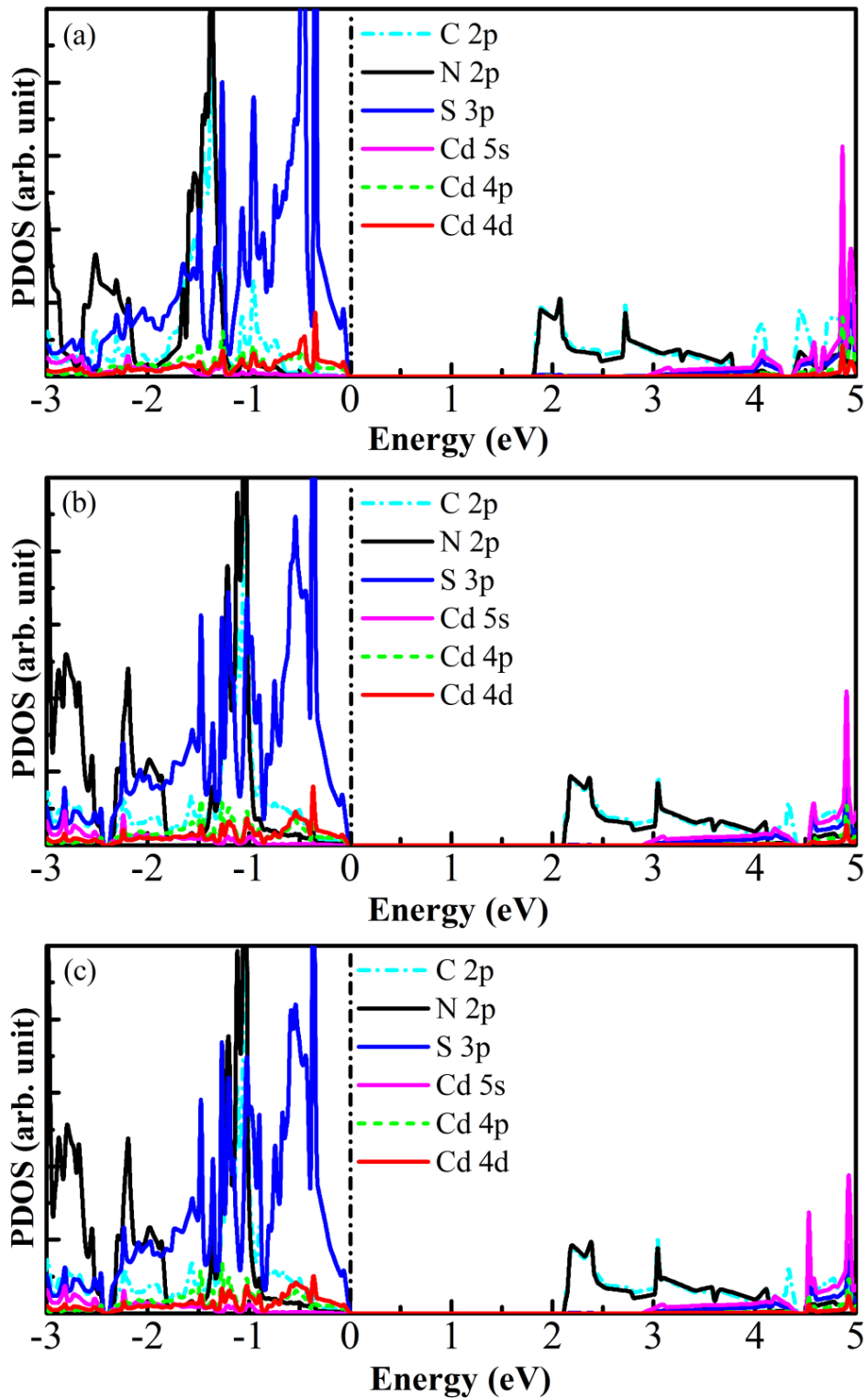
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1. The total and projected density of states for CdS monolayer and C<sub>2</sub>N monolayer are plotted in Figure S1.



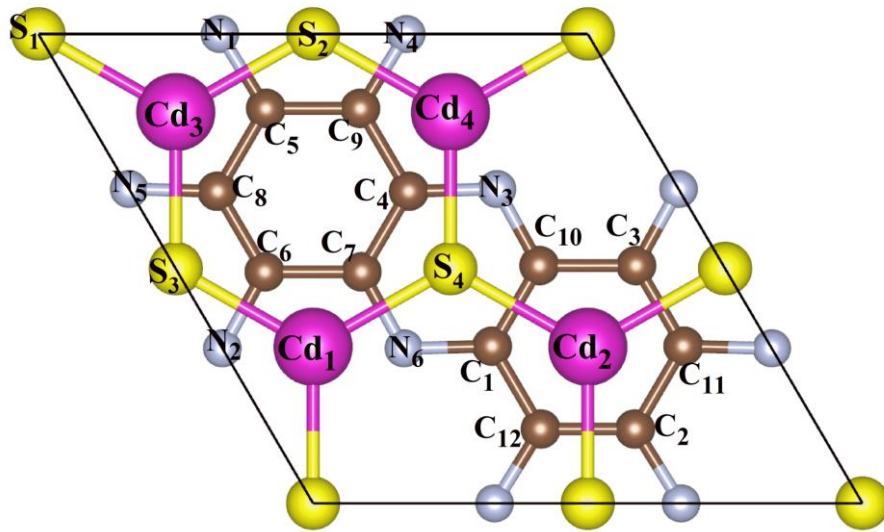
**Figure S1** (a) The calculated DOS and PDOS of CdS monolayer. (b) DOS and PDOS of C<sub>2</sub>N monolayer. The vertical black dashed line denotes the Fermi level.

2. The calculated projected density of states (PDOS) of the CdS/C<sub>2</sub>N heterostructure with different interlayer rotation angles ( $\theta = 0^\circ, 60^\circ, 120^\circ$ ) in Figure S2.



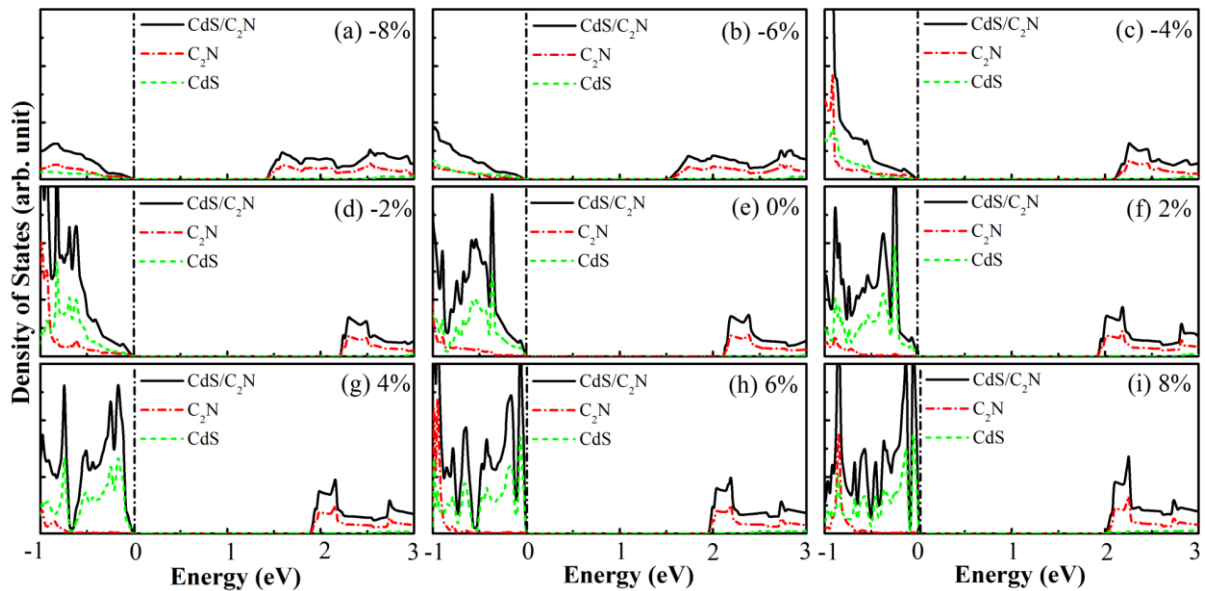
**Figure S2** The calculated PDOS of the CdS/C<sub>2</sub>N heterostructure with interlayer rotation angles of (a)  $0^\circ$ , (b)  $60^\circ$ , and (c)  $120^\circ$ . The vertical black dashed line indicates the Fermi level.

3. The numbering of atoms in the CdS/C<sub>2</sub>N heterostructure have been indicated in Figure S3



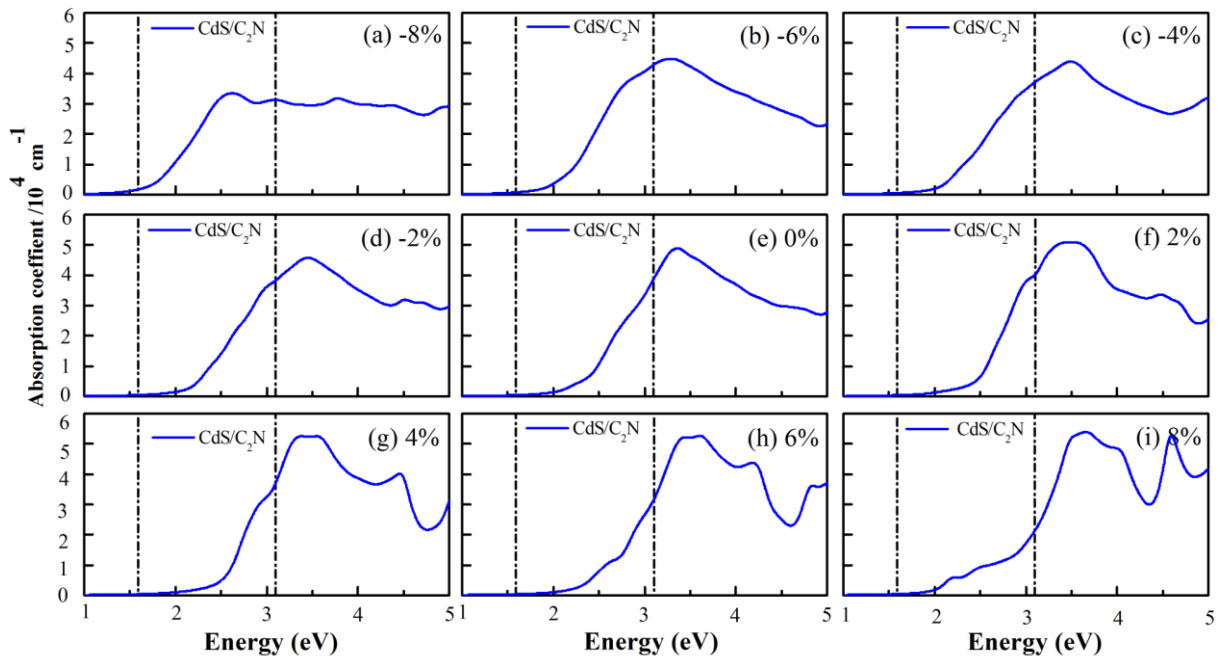
**Figure S3** The numbering of atoms in the CdS/C<sub>2</sub>N heterostructure.

4. The calculated density of states of the CdS/C<sub>2</sub>N heterostructure with different strains in Figure S4.



**Figure S4** The calculated DOS of the CdS/C<sub>2</sub>N heterostructure with strains of (a) -8%, (b) -6%, (c) -4%, (d) -2%, (e) 0%, (f) 2%, (g) 4%, (h) 6%, and (i) 8%. The vertical black dashed line indicates the Fermi level.

5. The calculated optical adsorption spectra of the CdS/C<sub>2</sub>N heterostructure with different strains in Figure S5.



**Figure S5** The calculated optical adsorption spectra of the CdS/C<sub>2</sub>N heterostructure with strains of (a) -8%, (b) -6%, (c) -4%, (d) -2%, (e) 0%, (f) 2%, (g) 4%, (h) 6%, and (i) 8%. The part between two vertical black dashed lines indicate the range of visible light.