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Supporting Information

Construction of heterojunction with fast charge transport channel for photocatalytic hydrogen evolution via a synergistic strategy of Co-doping and crystal plane modulation

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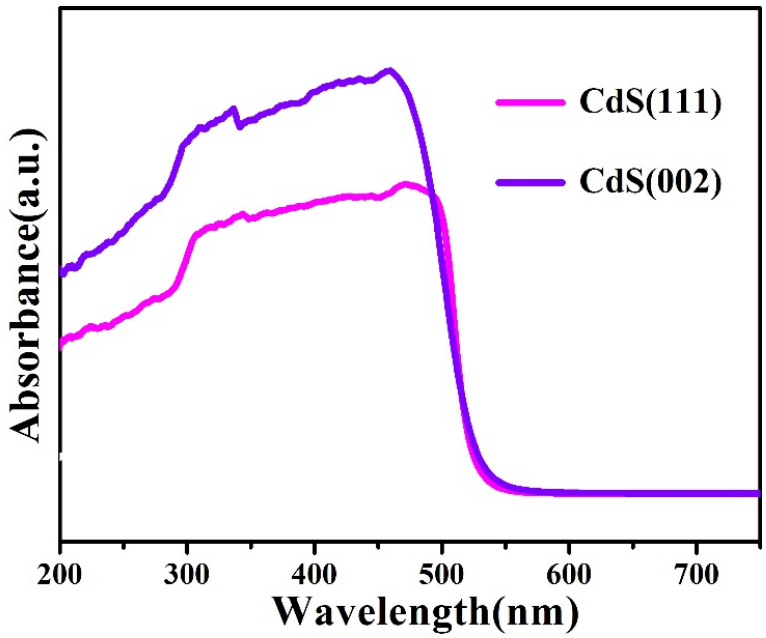

Fig. S1. UV-vis spectra of CdS(111) and CdS(002).

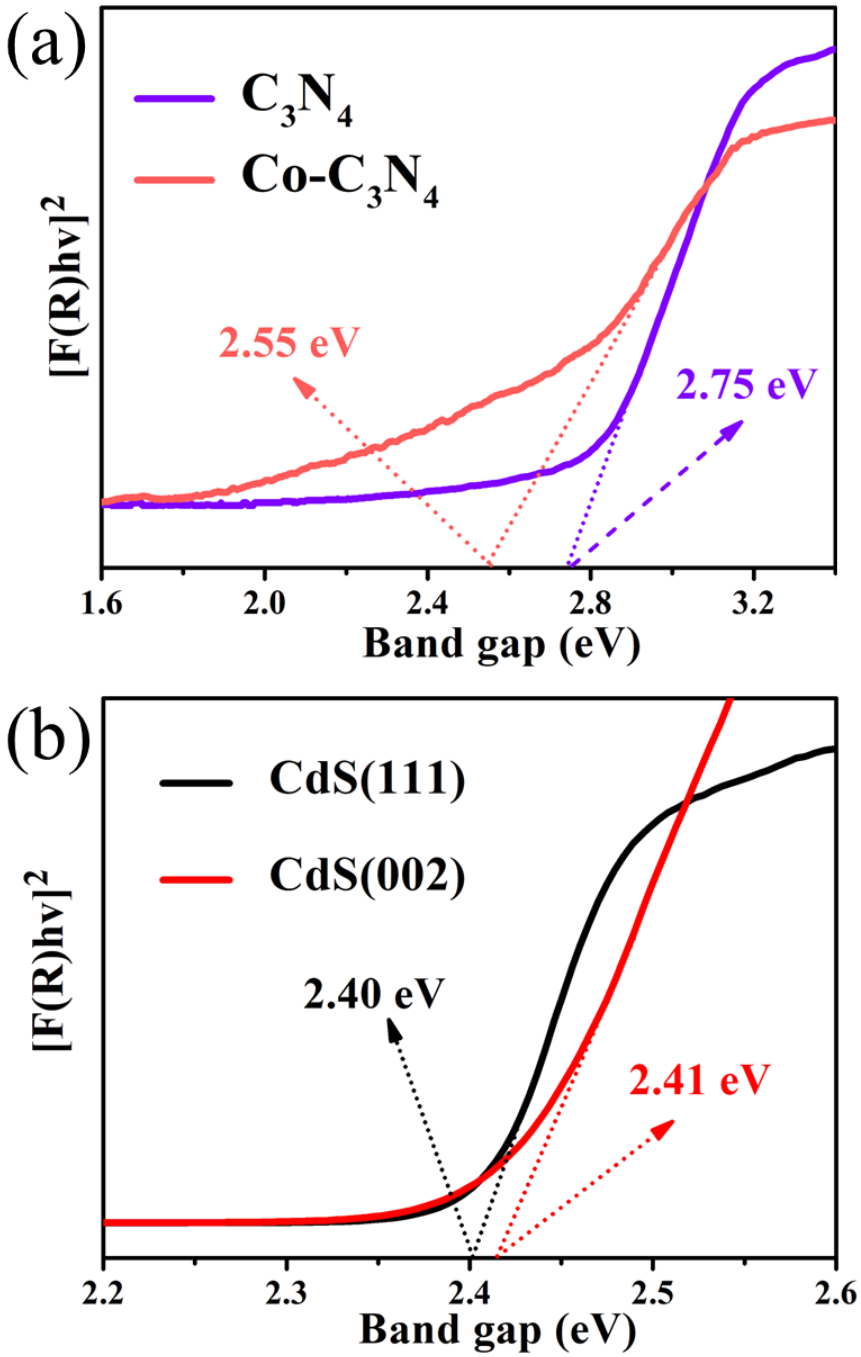

Fig. S2. Calculated Kubelka-Munk plots of (a) C_3N_4, Co-C_3N_4; (b) CdS(111), CdS(002).

Table S1. Information for BET specific surface area, pore diameter and pore volume.

Sample	S_{BET} (m^2 g^{-1})	Pore diameter (nm)	Pore volume (cm^3 g^{-1})
C_3N_4	121	11.51	0.295
Co-C_3N_4	135	9.09	0.321
CdS(111)/Co-C_3N_4	113	10.52	0.337
CdS(002)/Co-C_3N_4	118	12.13	0.359

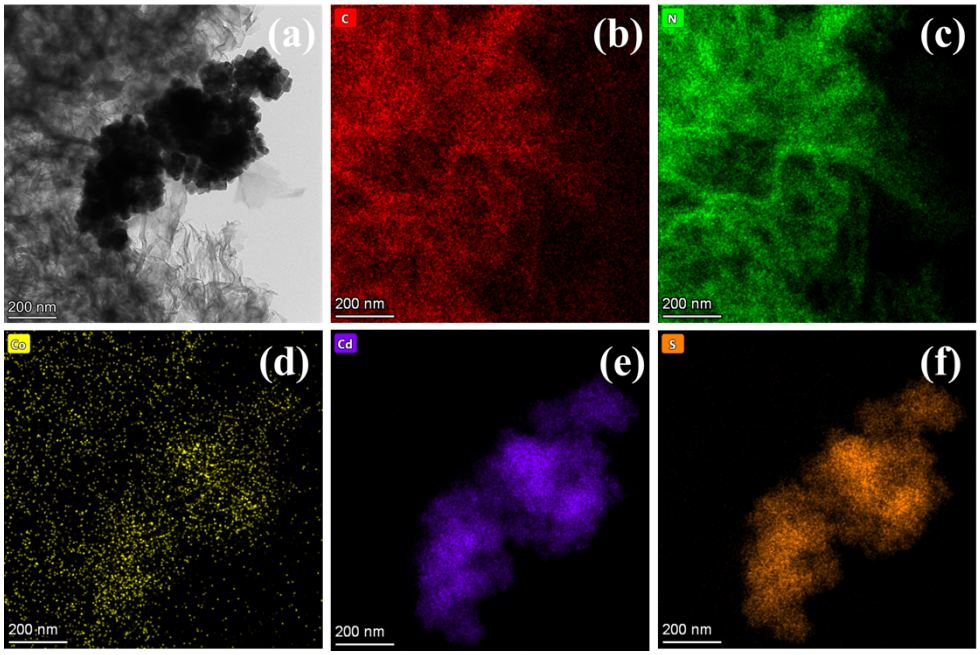

Fig. S3. (a) TEM images and (b-f) elemental mapping images of CdS(111)/Co-C_3N_4.

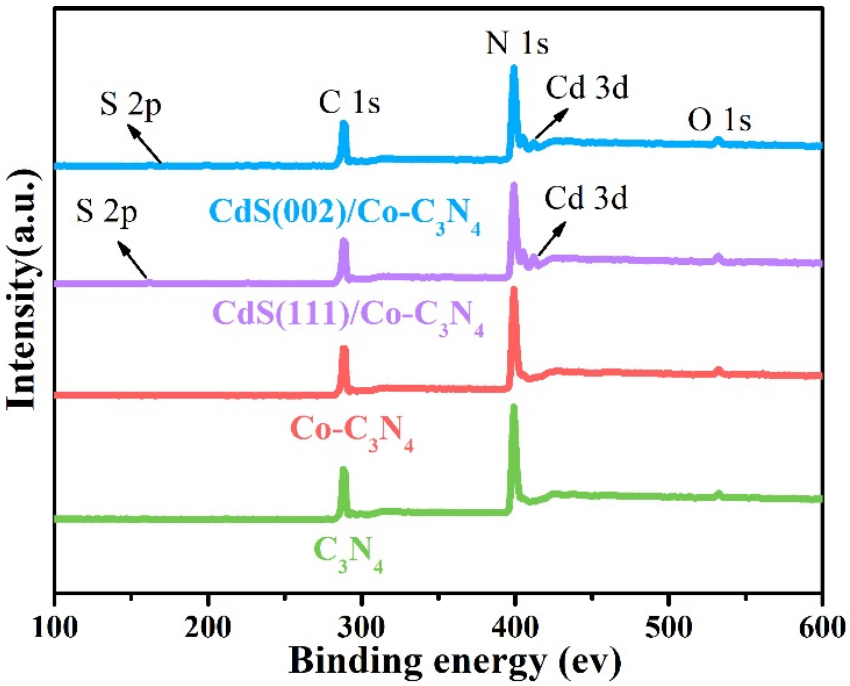

Fig. S4. Full x-ray photoelectron spectra.

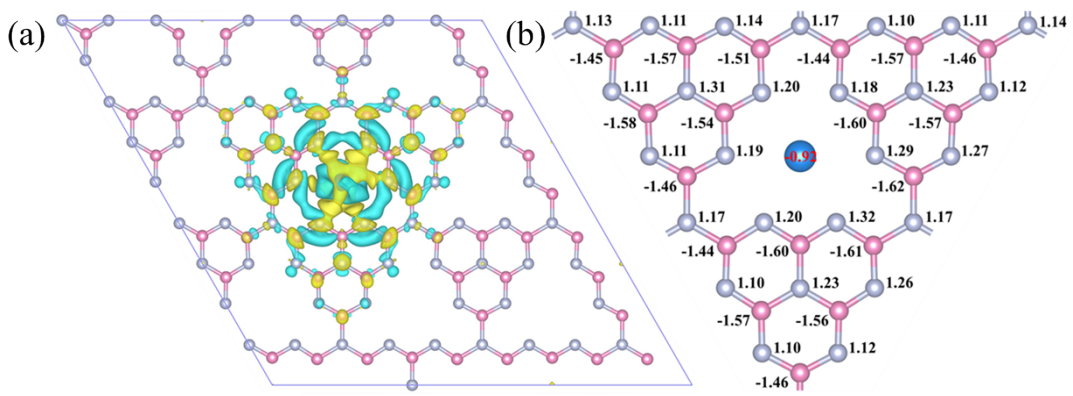

Fig. S5. (a) Top view of differential charge density of Co-C_3N_4, isosurface is 0.01 e/Å^3), yellow represents charge accumulation and cyan represents charge depletion; (b) Bader charge analysis.

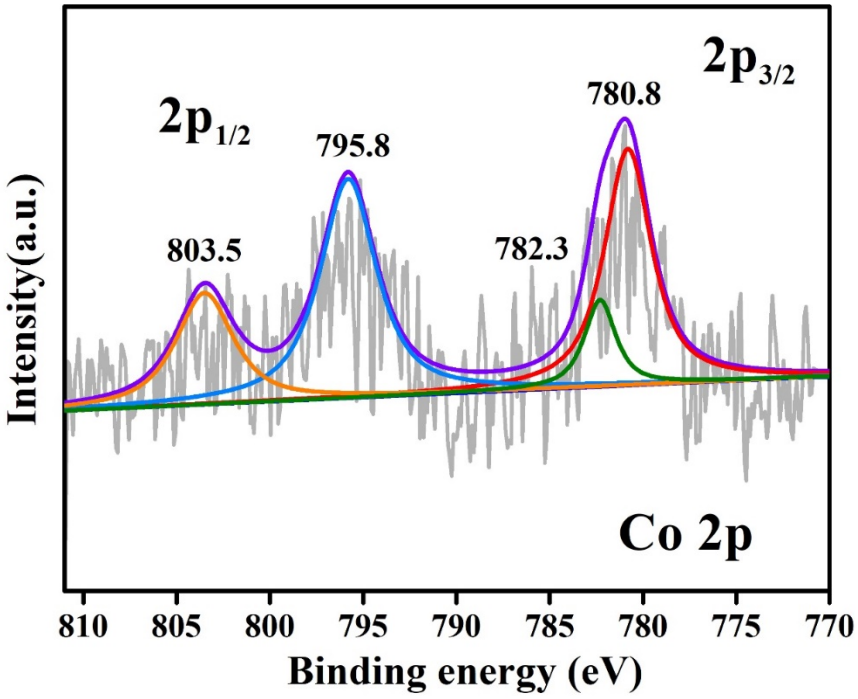

Fig. S6. X-ray photoelectron spectroscopy of Co 2p in Co-C_3N_4.

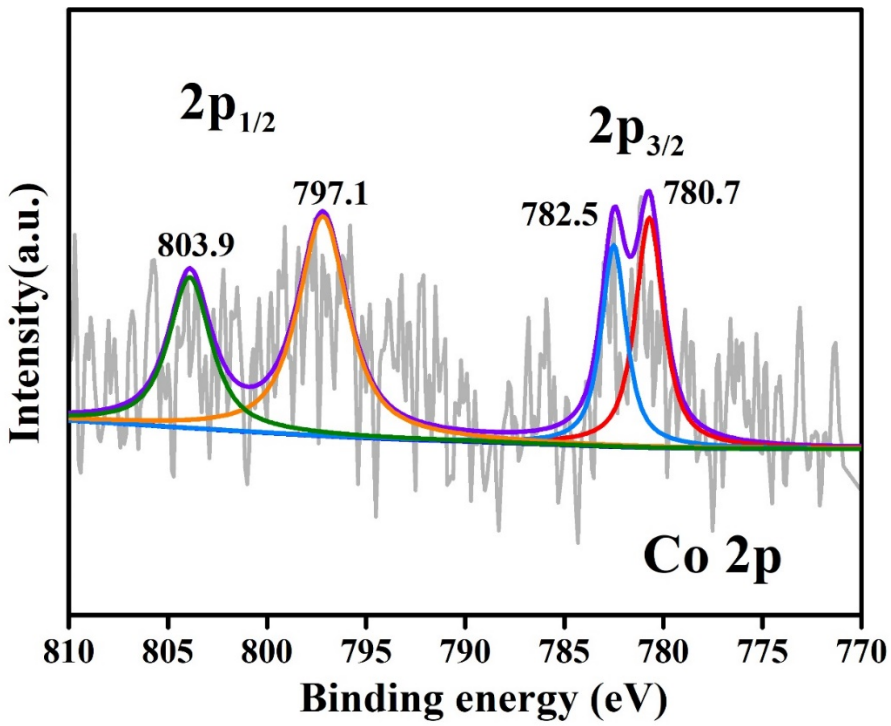

Fig. S7. X-ray photoelectron spectroscopy of Co 2p in CdS(111)/Co-C_3N_4.

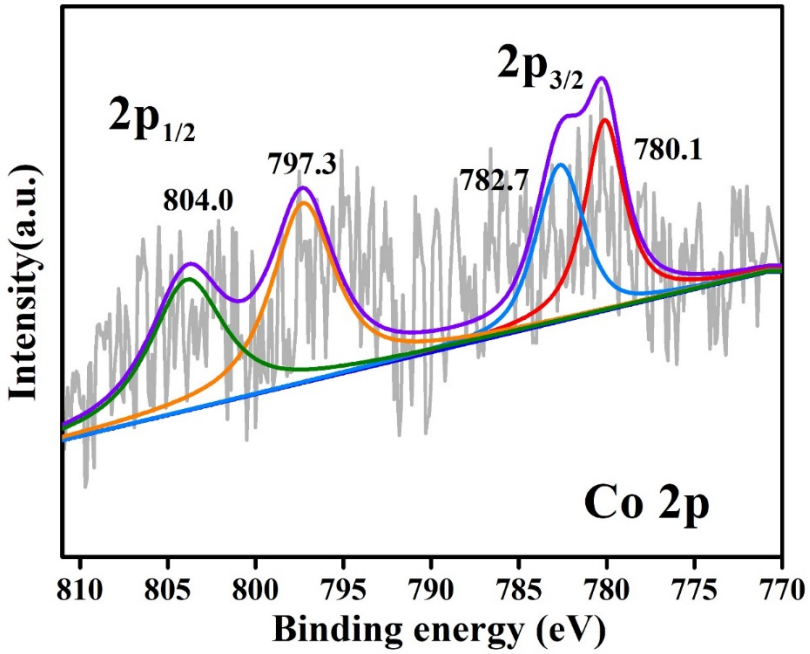

Fig. S8. X-ray photoelectron spectroscopy of Co 2p in CdS(002)/Co-C_3N_4.

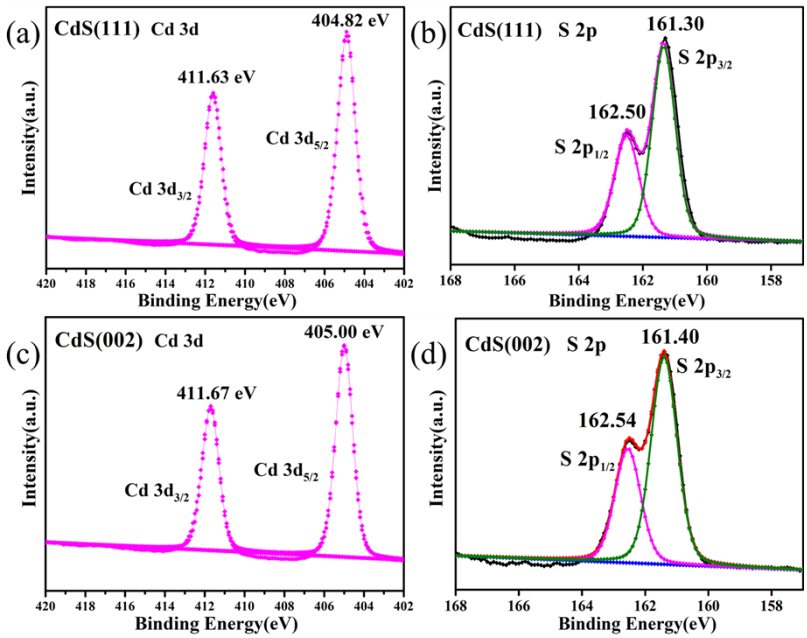

Fig. S9. (a, b) Cd 3d and S 2p spectra of CdS(111); (c, d) Cd 3d and S 2p spectra of CdS(002).

Table S2. Summary on the hydrogen evolution activity of the reported literature.

Photocatalyst	H_2 rate ($\mu mol\ h^{-1}\ g^{-1}$)	Sacrificial agents	Incident light λ (nm)	Amount (mg)	Pt (%)	Ref.
1wt%C-ZIF/g-C_3N_4	326	TEOA	> 400	100	-	[1]
g-C_3N_4/CoP-4%	936	TEOA	-	10	-	[2]
Pt/g-C_3N_4	665	TEOA	-	10	4	[2]
(Pt/MoP)/g-C_3N_4	531	TEOA	> 420	50	1	[3]
3.0%Pt/g-C_3N_4	287	TEOA	> 420	50	3	[3]
g-C_3N_4	803	TEOA	> 420	50	3	[4]
10%SiO_2-CN	248	TEOA	> 420	50	3	[5]
CN-2	925	lactic acid	> 420	20	1	[6]
CNsF-6%	54	-	> 420	100	-	[7]
BCN@Pt	893	methanol	> 420	30	0.5	[8]
$Ni(OH)_2$/2D-CN	921	TEOA	> 400	10	-	[9]
NiL/CN	468	TEOA	> 420	50	-	[10]
CdS(002)/Co-C_3N_4	991	TEOA	> 420	50	-	**This work**
CdS(002)/Co-C_3N_4	2337	lactic acid	> 420	50	-	**This work**

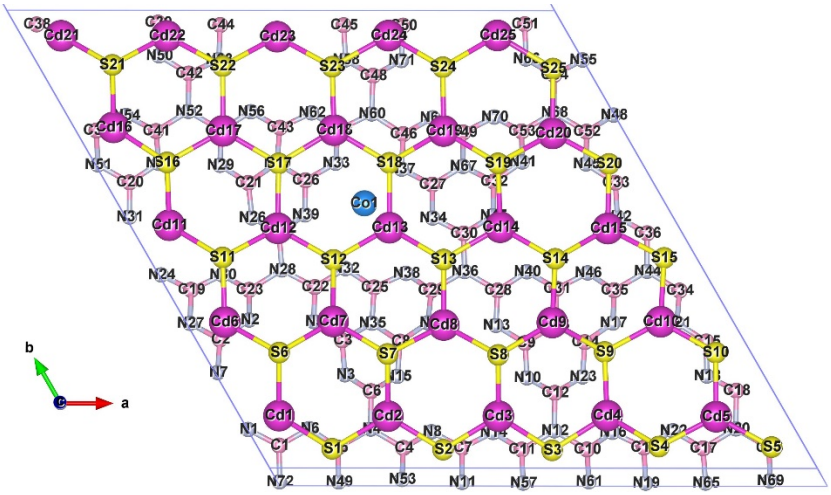

Fig. S10. Bader charge calculation model of CdS(002)/Co-C_3N_4.

Table S3. Bader charge analysis data for CdS(002)/Co-C_3N_4.

#	X	Y	Z	CHARGE	MIN DIST	ATOMIC VOL
1	0.069018	2.520616	5.247396	11.15719	1.043205	45.612622
2	4.249752	2.516327	4.930201	11.15307	1.076708	40.02962
3	8.50197	2.520963	4.890398	11.15833	1.049745	44.739533
4	12.67762	2.554897	4.632355	11.12759	1.05424	34.612754
5	16.8866	2.49424	5.366785	11.1817	1.065255	57.631383
6	-2.01943	6.108665	5.352237	11.15897	1.046607	42.131305
7	2.143424	6.141375	5.271211	11.18201	1.063055	51.226411
8	6.397212	6.016028	5.053744	11.11593	1.055611	26.537703
9	10.57495	6.110162	5.21828	11.18505	1.03613	54.740839
10	14.73405	6.16171	4.6473	11.14775	1.050743	47.925754
11	-4.16829	9.836298	5.027466	11.14294	1.063059	39.754274
12	0.001307	9.724148	5.06681	11.15635	1.063822	49.434344
13	4.297387	9.753025	4.951992	11.1826	1.063547	54.630468
14	8.567173	9.765237	5.28649	11.15932	1.056251	30.676595
15	12.69999	9.733658	4.888854	11.15556	1.05718	43.796156
16	-6.31615	13.58304	5.309679	11.13884	1.076279	44.406098
17	-2.09825	13.44716	5.498489	11.16047	1.051894	69.467742
18	2.162046	13.49068	5.141094	11.1733	1.070595	54.419022
19	6.385303	13.4537	5.39897	11.1807	1.058156	55.439077
20	10.57318	13.37482	5.153096	11.15172	1.050917	45.714279
21	-8.33873	17.10374	5.136565	11.17947	1.035959	39.618344
22	-4.27619	17.09711	5.296696	11.15581	1.068394	43.600394
23	-0.03499	17.08267	5.026193	11.13763	1.047529	38.392071
24	4.257329	17.11708	5.365909	11.15877	1.061597	39.962816
25	8.441952	17.13274	5.235395	11.1316	1.103449	37.351684
26	2.105664	1.274154	4.50994	6.841972	1.127949	44.82144
27	6.371382	1.243031	4.58318	6.853033	1.16279	47.596966
28	10.56215	1.228629	4.384915	6.84324	1.123457	45.868797
29	14.68918	1.340578	5.497257	6.816865	1.119031	143.645979
30	19.03065	1.317853	5.790032	6.828712	1.143866	151.169758
31	0.080431	4.920467	5.917832	6.809988	1.111755	178.410928
32	4.247381	4.87978	5.687341	6.820831	1.126083	161.902994
33	8.504931	4.845682	5.734741	6.807242	1.127604	181.092349
34	12.56921	5.014291	4.209651	6.820119	1.113513	44.50427
35	16.86259	4.967306	5.100059	6.864019	1.116349	85.777009
36	-2.10252	8.579741	5.66173	6.821264	1.129609	156.727782
37	2.140747	8.529489	4.52455	6.855913	1.141686	48.269645
38	6.391384	8.516091	5.408885	6.829129	1.125529	121.570727
39	10.69434	8.540952	5.725328	6.81585	1.124098	182.157714
40	14.85426	8.627766	4.283289	6.83541	1.116661	44.1354

41	-4.24782	12.22618	5.715205	6.825338	1.161064	142.855378
42	0.035347	12.21561	5.061759	6.845432	1.148396	68.573742
43	4.288619	12.2496	4.785181	6.838832	1.146462	55.117841
44	8.484265	12.20251	5.826767	6.820158	1.108419	175.920041
45	12.73287	12.22085	4.706264	6.851125	1.11986	50.967912
46	-6.34691	15.95781	6.068738	6.78785	1.103391	214.672849
47	-2.11359	15.92483	5.734073	6.838868	1.136817	158.00227
48	2.100395	15.91402	5.558517	6.841335	1.123144	140.630542
49	6.358535	15.89369	5.792015	6.825251	1.135377	148.786338
50	10.5867	15.86675	5.141533	6.811023	1.159158	70.554601
51	0.007746	1.498161	1.449073	2.529147	0.400529	14.129741
52	-2.26955	5.555363	1.874031	2.580964	0.360232	8.506076
53	2.417399	5.552643	1.004829	2.48358	0.334469	14.896525
54	4.782884	1.414761	1.264626	2.522123	0.40166	7.522037
55	2.264661	1.4294	1.144235	2.570756	0.370355	12.343483
56	3.536851	3.59117	1.329058	2.517916	0.342166	7.581869
57	7.04354	1.437906	0.914161	2.502341	0.364762	18.049635
58	4.661931	5.476233	1.993462	2.495216	0.352649	7.605686
59	9.471667	5.436368	1.675265	2.577028	0.389418	12.177346
60	11.84512	1.369711	1.126452	2.519105	0.391273	6.995163
61	9.333009	1.365732	1.011342	2.505897	0.392964	10.186612
62	10.60465	3.541009	1.09794	2.464236	0.336267	7.307686
63	14.04657	1.423449	1.77422	2.495906	0.392322	10.070432
64	11.74905	5.502792	0.783584	2.451292	0.36202	16.82278
65	16.43215	5.511956	1.452893	2.289265	0.371402	8.27546
66	18.8619	1.414377	1.956268	2.52258	0.390278	8.026836
67	16.32415	1.38906	1.968395	2.581952	0.36369	11.290897
68	17.6001	3.6082	1.927339	2.460347	0.338386	7.372165
69	-3.3994	7.492267	0.852483	2.525526	0.383554	18.578832
70	-5.76421	11.60062	1.344733	2.421355	0.39019	11.663833
71	-1.18788	11.56608	1.936001	2.493141	0.34455	7.552243
72	1.363803	7.596531	1.092555	2.574241	0.427736	8.388154
73	-1.15666	7.47728	1.308854	2.554733	0.339747	7.389592
74	-0.01247	9.690726	1.308457	2.511486	0.361328	7.110761
75	3.652492	7.578862	1.332085	2.405317	0.363512	12.281908
76	0.992198	11.70119	0.939291	2.498712	0.322622	24.438341
77	5.887698	11.51362	1.761134	2.37188	0.35166	9.208962
78	8.411527	7.443986	1.982233	2.515825	0.445015	11.510476
79	5.856904	7.445264	1.933559	2.605693	0.345343	8.123265
80	7.103442	9.621308	2.187615	2.591722	0.366742	8.259195
81	10.67866	7.525853	1.630348	2.434367	0.331651	13.752739
82	8.257883	11.61841	2.127649	2.492003	0.352576	8.754119
83	12.91837	11.6206	0.980263	2.55568	0.366258	20.934951

84	15.38955	7.480548	0.943549	2.566355	0.412579	9.068966
85	12.87434	7.489273	1.000279	2.52805	0.335688	7.590002
86	14.14142	9.681471	0.928041	2.593051	0.365632	12.223818
87	-7.03272	13.57147	1.939779	2.481279	0.359041	7.920532
88	-9.35632	17.67069	1.086064	2.483528	0.355044	19.134751
89	-4.67245	17.72365	1.772238	2.505692	0.403977	8.971956
90	-2.23216	13.58197	2.200723	2.631578	0.418847	7.929245
91	-4.74194	13.55048	1.961987	2.518521	0.323826	8.590306
92	-3.48489	15.76409	1.926462	2.509501	0.365486	9.019008
93	0.02621	13.68957	1.893067	2.444765	0.34288	8.063433
94	-2.28747	17.64576	1.399982	2.425477	0.378904	16.893069
95	2.449689	17.66377	0.862084	2.453204	0.340228	18.978489
96	4.756252	13.47286	1.199484	2.560312	0.407241	10.759957
97	2.24507	13.62393	1.280113	2.6223	0.363292	7.705019
98	3.59102	15.71227	1.197167	2.503197	0.350308	7.954224
99	7.066567	13.53861	1.15129	2.459095	0.356544	22.603868
100	4.753375	17.62192	1.643498	2.426856	0.372065	13.153834
101	9.438354	17.67047	1.968729	2.523485	0.35074	8.129655
102	11.81303	13.56289	1.475873	2.557035	0.413812	7.178726
103	9.313945	13.5676	1.556482	2.500277	0.333254	7.249015
104	10.56306	15.73799	1.500669	2.485335	0.327748	7.16827
105	-1.18497	2.110842	1.480528	6.160534	0.712648	79.40573
106	-1.14203	6.300783	1.953701	6.136948	0.733151	19.672661
107	2.519076	4.24054	0.763171	6.121447	0.684046	112.141605
108	3.525775	2.143315	1.215367	6.098514	0.756507	20.918105
109	1.320267	6.280832	0.807942	6.146195	0.704535	84.407835
110	1.160901	2.148591	1.379485	6.100629	0.677719	23.117381
111	-2.3446	4.272228	2.253008	6.088077	0.691826	17.412972
112	5.855375	2.053727	0.771937	6.11431	0.672522	105.316064
113	5.746268	6.185147	2.415686	6.097099	0.704516	16.125704
114	9.538967	4.100645	1.688519	6.08011	0.678008	18.822809
115	7.044626	0.09658	1.337678	6.21716	0.753421	28.656816
116	10.59029	2.090234	1.021235	6.119128	0.773417	22.383708
117	8.349064	6.105324	1.975408	6.172809	0.660943	25.632085
118	8.219364	2.035857	0.658434	6.116237	0.670612	119.718246
119	4.5639	4.142628	2.034893	6.127822	0.72147	18.255853
120	12.83451	2.008951	1.78593	6.122315	0.690746	16.552082
121	12.82425	6.251189	0.477347	6.124272	0.737446	137.931113
122	16.45797	4.181672	1.557567	6.224595	0.671464	59.622698
123	14.10716	0.072302	1.402007	6.176556	0.748681	25.004135
124	17.58705	2.138442	2.019573	6.049096	0.74596	17.932875
125	15.30172	6.225177	1.406202	6.189446	0.737141	19.046454
126	15.16831	2.056812	2.131511	6.112361	0.671966	17.859101

127	11.66001	4.178989	0.557643	6.185663	0.769507	105.176649
128	-4.55892	8.075669	0.513999	6.057778	0.685168	130.897611
129	-4.64083	12.33165	1.430664	6.115649	0.74195	77.023471
130	-1.04246	10.22406	1.985468	6.127679	0.633485	18.142578
131	-3.42824	6.189163	1.383368	6.248698	0.715973	24.052045
132	0.098874	8.250428	1.249264	6.067735	0.752371	17.591888
133	-2.26945	12.23128	2.305376	6.090202	0.664884	16.990659
134	-2.19555	8.073186	0.702308	6.105084	0.664697	102.882686
135	-5.77036	10.27548	1.218498	6.167531	0.74908	22.601545
136	2.539626	8.303528	1.184414	6.171669	0.736832	32.810811
137	2.151781	12.36706	0.738625	6.148161	0.738396	93.169506
138	5.906646	10.22397	2.0652	6.177197	0.681558	16.384784
139	3.570269	6.20174	1.494178	6.160326	0.735502	14.853539
140	7.137746	8.168817	2.074258	5.978782	0.761109	17.210239
141	4.698679	12.11792	1.490588	6.155755	0.701182	18.902973
142	4.877089	8.120226	1.327848	6.205377	0.664536	96.376058
143	0.979941	10.38283	0.710907	6.179157	0.725121	101.200989
144	9.536217	8.166499	1.908283	6.106152	0.66987	28.186289
145	9.351874	12.37511	2.202121	6.180307	0.736263	17.928808
146	12.98823	10.32082	0.649439	6.055934	0.683148	117.206447
147	10.63072	6.154992	1.344044	6.173728	0.715949	25.736065
148	14.13918	8.224691	0.890283	5.98099	0.766396	24.933266
149	11.78586	12.34326	0.917709	6.10693	0.68158	96.827996
150	11.87195	8.135686	1.613066	6.182813	0.68246	19.326447
151	8.236742	10.30317	2.428668	6.11811	0.725497	17.323513
152	12.86367	14.18231	2.038776	6.12556	0.667548	18.490536
153	2.292894	0.123631	0.819171	6.115377	0.726937	119.230874
154	-4.6249	16.43827	2.169102	6.104924	0.667261	21.422323
155	-6.98718	12.27563	1.403134	6.224045	0.780863	28.217658
156	-3.48994	14.3053	2.102018	6.046655	0.744369	17.089993
157	4.740919	0.191808	1.809787	6.104653	0.705921	18.947121
158	-5.8838	14.13494	2.370331	6.146119	0.672739	18.147806
159	11.64594	16.33395	0.977737	6.130488	0.758046	90.436385
160	-1.08966	14.28929	2.276531	6.140925	0.662917	17.149244
161	9.395061	0.070203	1.34538	6.146988	0.768654	21.273614
162	2.523998	16.33851	0.663026	6.173463	0.682802	111.729168
163	-0.09987	12.34346	1.430956	6.215422	0.727035	44.270749
164	3.539359	14.24694	1.211652	6.12439	0.787986	19.500716
165	11.90788	0.152582	0.571335	6.123303	0.652067	134.938912
166	1.244104	14.26167	1.888663	6.18356	0.65652	18.941312
167	-2.33715	16.31296	1.529891	6.173891	0.760294	54.29471
168	5.890143	14.1092	0.900406	6.127546	0.663177	101.616912
169	16.41775	0.063942	1.804965	6.126169	0.77395	39.426067

170	9.486211	16.33659	2.040508	6.105387	0.637186	18.658415
171	7.066104	12.2195	1.666979	6.268142	0.721579	27.635599
172	10.56126	14.29238	1.501776	6.062463	0.738292	16.399887
173	18.90791	0.132649	2.366052	6.134868	0.645552	16.95232
174	8.254226	14.13808	0.975337	6.192697	0.675148	103.20218
175	4.690364	16.28322	1.69691	6.179957	0.731684	21.242245
176	0.028096	0.103863	1.500607	6.152361	0.722922	17.648235
177	3.267671	10.81228	1.189214	8.145887	0.840612	64.807205

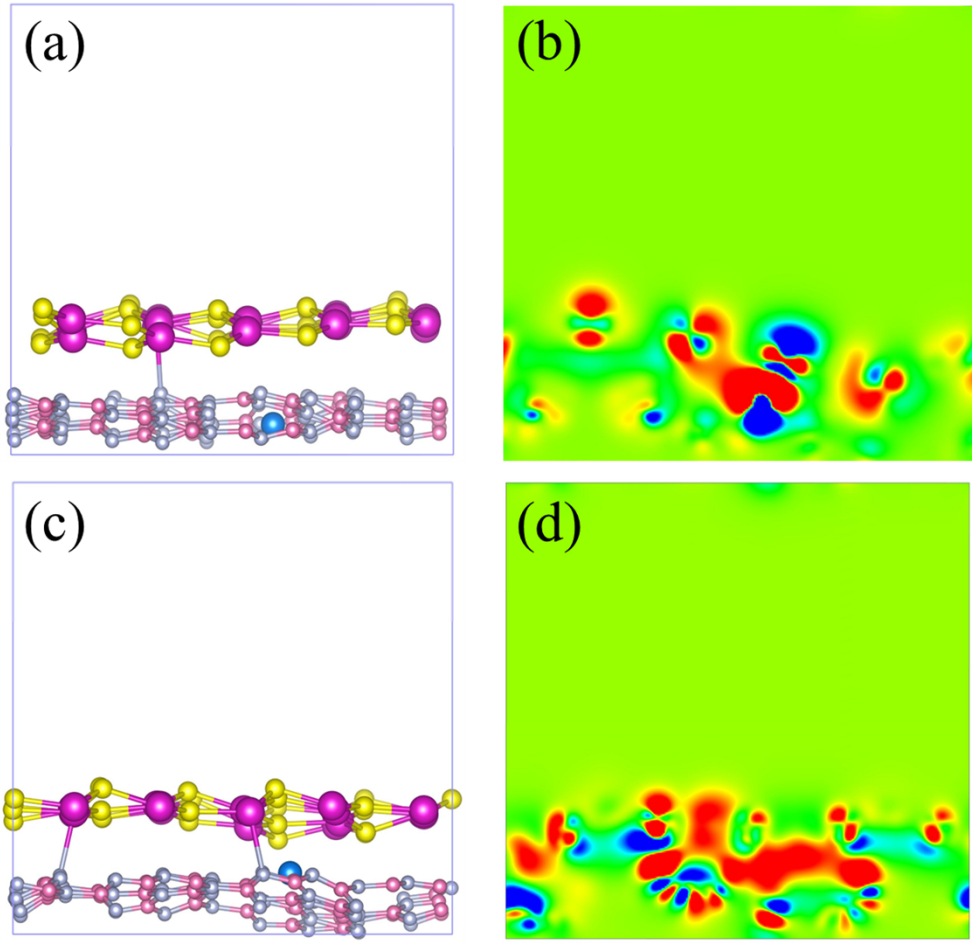

Fig. S11. (a) side view of the optimized model of CdS(111)/Co-C_3N_4; (b) 2D date display charge density distribution image of CdS(111)/Co-C_3N_4; (c) side view of the optimized model of CdS(002)/Co-C_3N_4; (d) 2D date display charge density distribution image of CdS(002)/Co-C_3N_4. C, N, Co, Cd, S atoms are shown in pink, light purple, dark blue, rosy red and yellow, respectively. Red represents electron-rich regions and blue represents electron-deficient regions.

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