Supplementary Information (SI) for Physical Chemistry Chemical Physics.

Electronic transitions and vibrational properties in bulk and monolayer g-C_3N_4, and g-C_3N_4/MoS_2 heterostructure from DFT study.

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Supporting information

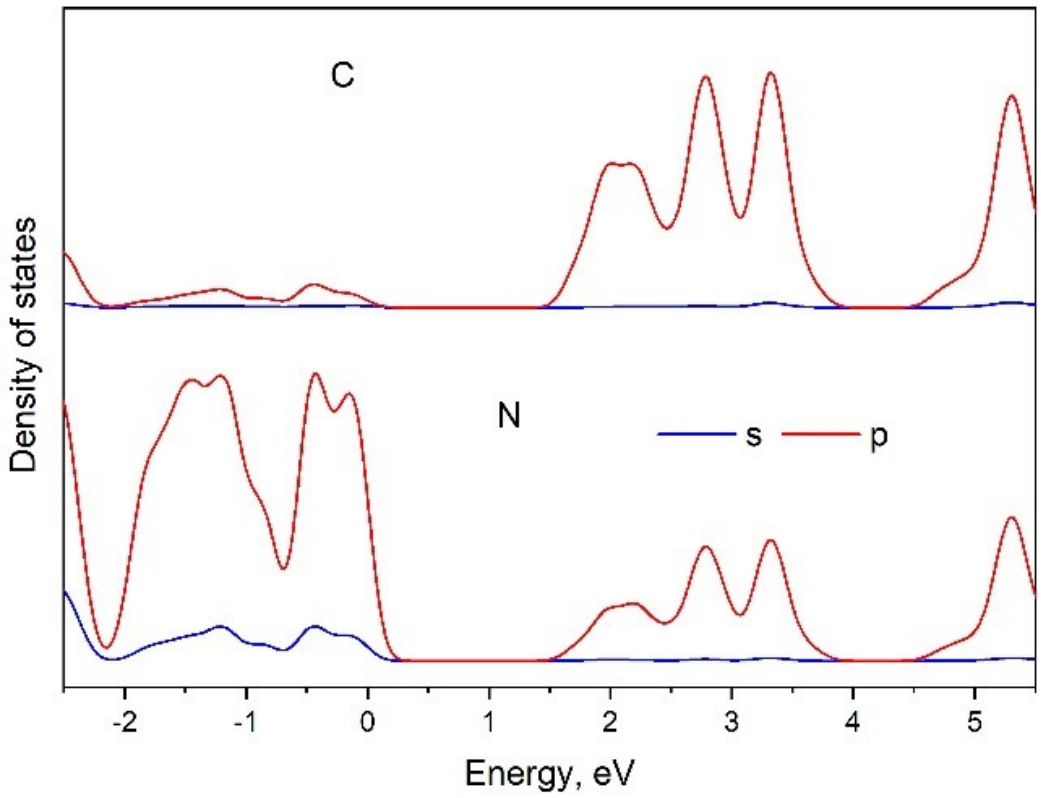

Figure S1. Density of states of the bulk “phase 1” g-C_3N_4.

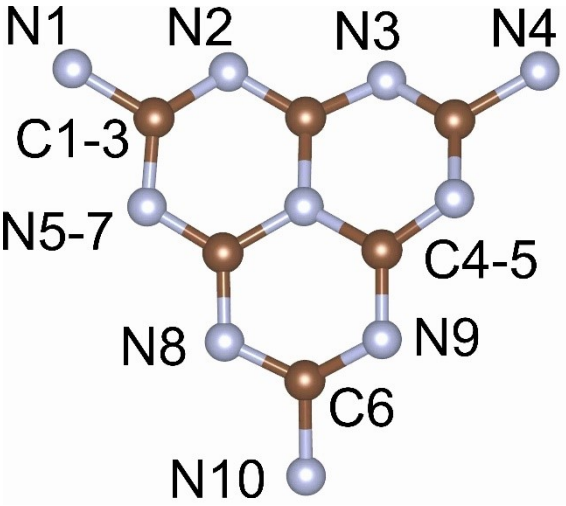

Figure S2. Designations of N and C ions in a structural triangle.

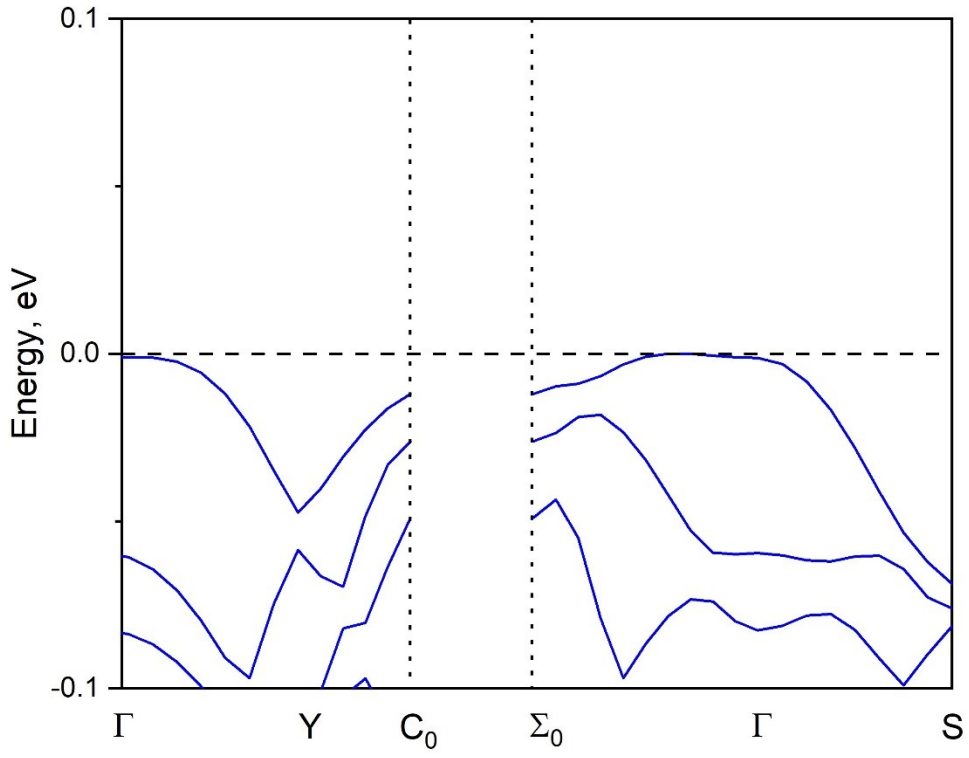

Figure S3. Electronic band structure of the g-C_3N_4/MoS_2 heterostructure in the vicinity of the top of the valence band.

Table S1. Structural parameters for the bulk g-C_3N_4 after PBE-TS optimization.

	a	b	c
cell length	6.9751	6.9751	6.7393
	alpha	betta	Gamma
angle	90	90	119.7165
	fractional coordinates		
atom	x	y	z
N	-0.35674	-0.98676	1.08120
N	-0.99422	-0.29558	0.90403
N	-0.68057	-0.65117	0.98830
N	-0.01953	-0.98047	1.00000
N	-0.68312	-0.31688	1.00000
C	-0.90297	-0.42307	0.93822
C	-0.25444	-0.10057	1.02776
C	-0.89811	-0.10189	1.00000
C	-0.56763	-0.43237	1.00000

Table S2. Structural parameters for the monolayer g-C_3N_4 after PBE-TS optimization.

	a	b	c
cell length	6.9457	6.9455	26.1962
	alpha	betta	Gamma
angle	90.7035	90.8741	119.7053
	fractional coordinates		
atom	x	y	z
N	0.99098	0.28179	0.09768
N	0.01675	0.63581	0.10266
N	0.68411	0.64729	0.12013
N	0.02520	0.97479	0.12516
N	0.68791	0.31204	0.12515
N	0.35275	0.31582	0.13016
N	0.36436	0.98311	0.14772
N	0.71843	0.00883	0.15270
C	0.90544	0.41500	0.10744
C	0.90405	0.74014	0.11635
C	0.90316	0.09685	0.12518
C	0.57131	0.42869	0.12516

C	0.25993	0.09588	0.13399
C	0.58514	0.09443	0.14293

Table S3. Comparison of bond lengths in the bulk structure and monolayer.

	Bond length		
Bond	Bulk	Monolayer	Delta
N1–C1	1.43551	1.42937	0.00614
C1–N2	1.35300	1.35313	-0.00013
N2–C2	1.34029	1.34086	-0.00057
C2–N3	1.34540	1.34839	-0.00299
N3–C3	1.33979	1.34195	-0.00216
C3–N4	1.46480	1.46601	-0.00121
C1–N5	1.33385	1.33754	-0.00369
C2–N6	1.39551	1.40295	-0.00744
C3–N7	1.33979	1.34209	-0.0023
N5–C4	1.32816	1.32869	-0.00053
C4–N6	1.39326	1.40096	-0.0077
N6–C5	1.39551	1.40321	-0.0077
C5–N7	1.34540	1.34838	-0.00298
C4–N8	1.32816	1.32865	-0.00049
C5–N9	1.34029	1.34092	-0.00063
N8–C6	1.33385	1.33748	-0.00363
N9–C6	1.35300	1.35314	-0.00014
C6-N10	1.43551	1.42957	0.00594

Table S4. Structural parameters for the g-C_3N_4/MoS_2 after PBE-TS optimization.

	a	b	c
cell length	13.909838	36.799924	26.814604
	alpha	betta	Gamma
angle	87.613153	92.500255	160.835729
		fractional coordinates	
atom	x	y	z
C	0.339625	0.170847	0.437689
C	0.835025	0.169179	0.435816
C	0.336874	0.670174	0.437123
C	0.838495	0.670748	0.436821
C	0.497046	0.168522	0.444649
C	0.993763	0.167399	0.443214
C	0.494866	0.668072	0.444436
C	0.997780	0.669190	0.442805

C	0.171602	0.166986	0.452961
C	0.670328	0.166405	0.452803
C	0.169084	0.666359	0.452557
C	0.668792	0.666061	0.452909
C	0.007320	0.001939	0.450632
C	0.505009	0.001110	0.450668
C	0.005593	0.501644	0.450805
C	0.507966	0.502215	0.448499
C	0.029583	0.345567	0.459400
C	0.525974	0.344832	0.459102
C	0.026359	0.844717	0.459760
C	0.528257	0.845428	0.459547
C	0.348649	0.006131	0.469350
C	0.849963	0.006642	0.469364
C	0.350231	0.506514	0.469342
C	0.846531	0.505807	0.468736
N	0.361804	0.214841	0.428275
N	0.857029	0.213221	0.427185
N	0.358013	0.713817	0.427609
N	0.857760	0.713736	0.427695
N	0.055726	0.224597	0.430176
N	0.561957	0.226931	0.433849
N	0.062590	0.727721	0.433106
N	0.559246	0.726314	0.433104
N	0.228712	0.058108	0.445634
N	0.726845	0.057432	0.446307
N	0.227163	0.557841	0.445952
N	0.729566	0.558702	0.441812
N	0.230561	0.227203	0.451981
N	0.732518	0.227629	0.452724
N	0.231504	0.727690	0.452309
N	0.729945	0.727025	0.452639
N	0.066037	0.060094	0.452987
N	0.563867	0.059314	0.452436
N	0.063979	0.559682	0.452894
N	0.566164	0.560142	0.452227
N	0.232200	0.392667	0.451965
N	0.729588	0.392100	0.453594
N	0.228838	0.891567	0.453479
N	0.730683	0.892258	0.453255
N	0.075109	0.395989	0.474459
N	0.570011	0.395060	0.472955
N	0.072733	0.895542	0.474403
N	0.573894	0.896030	0.474069
N	0.434199	0.070826	0.478520

N	0.934674	0.071115	0.478415
N	0.433597	0.570530	0.478627
N	0.931091	0.570219	0.477884
S	0.972173	0.006337	0.317550
S	0.919949	0.216422	0.315997
S	0.708446	0.058632	0.316290
S	0.864228	0.426146	0.317226
S	0.656300	0.269376	0.316631
S	0.446628	0.111538	0.317423
S	0.811237	0.636697	0.316702
S	0.601433	0.478866	0.317463
S	0.390922	0.320910	0.316876
S	0.178958	0.162966	0.316254
S	0.762090	0.848317	0.317996
S	0.550395	0.689769	0.317077
S	0.339651	0.532080	0.317323
S	0.128714	0.374015	0.317217
S	0.498103	0.901019	0.317350
S	0.286230	0.742472	0.317709
S	0.074079	0.583641	0.317351
S	0.236289	0.953677	0.317464
S	0.026352	0.796411	0.316737
S	0.960964	0.005510	0.199489
S	0.909439	0.216798	0.198633
S	0.697877	0.058386	0.198287
S	0.858211	0.427678	0.198913
S	0.646533	0.269332	0.198965
S	0.434134	0.110839	0.199276
S	0.804150	0.637538	0.199208
S	0.594689	0.480123	0.199103
S	0.385732	0.322841	0.198598
S	0.172675	0.163926	0.198598
S	0.751099	0.848092	0.199773
S	0.541836	0.690710	0.199363
S	0.330759	0.532532	0.198975
S	0.119519	0.374347	0.198962
S	0.486852	0.899968	0.198949
S	0.278668	0.743019	0.199685
S	0.069190	0.585798	0.199568
S	0.223509	0.953117	0.199053
S	0.014502	0.795441	0.198794
Mo	0.789860	0.040528	0.257402
Mo	0.949618	0.409683	0.258033
Mo	0.738635	0.251522	0.258085
Mo	0.528269	0.093703	0.258022

Mo	0.896090	0.619669	0.258379
Mo	0.685477	0.461888	0.258198
Mo	0.475707	0.304257	0.257712
Mo	0.264928	0.146327	0.257969
Mo	0.844251	0.830690	0.258649
Mo	0.634283	0.672821	0.258052
Mo	0.421568	0.514280	0.258004
Mo	0.212871	0.357006	0.257999
Mo	0.002580	0.199105	0.257226
Mo	0.580294	0.883018	0.258584
Mo	0.371071	0.725493	0.259028
Mo	0.159382	0.567115	0.258297
Mo	0.317557	0.935879	0.257592
Mo	0.107428	0.778059	0.258134
Mo	0.054388	0.988325	0.258749