

Supporting information for:

First-principles calculations on the interfacial, electronic and photocatalytic properties of Ta₃N₅/SrTaO₂N heterostructure

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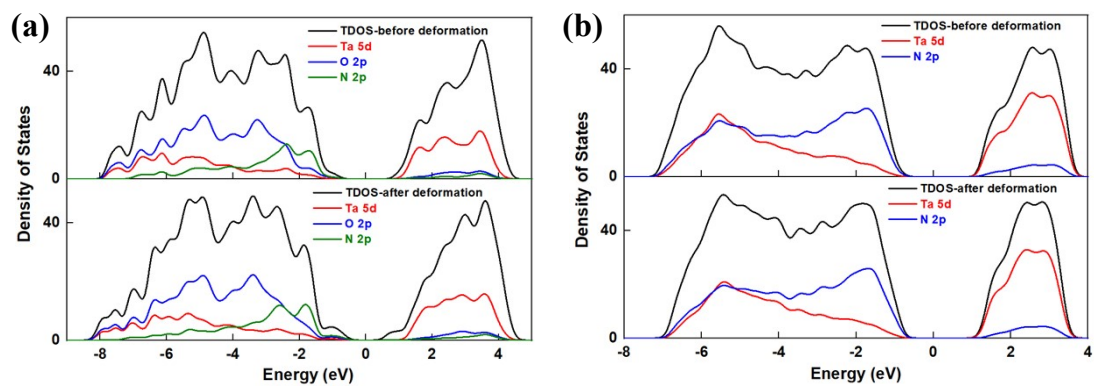


Fig. S1 Calculated DOS of (a) SrTaO₂N(001) and (b) Ta₃N₅(110) before and after deformation being subjected to strain.

The structural information of Ta₃N₅/Sr₂ON:

_cell_length_a		10.7926					
_cell_length_b		5.5644					
_cell_length_c		44.9259					
_cell_angle_alpha		90.0000					
_cell_angle_beta		90.0000					
_cell_angle_gamma		90.0000					
loop_							
_atom_site_label							
_atom_site_type_symbol							
_atom_site_fract_x							
_atom_site_fract_y							
_atom_site_fract_z							
_atom_site_U_iso_or_equiv							
_atom_site_adp_type							
_atom_site_occupancy							
Sr1	Sr	0.49970	0.51991	0.34456	0.01267	Uiso	1.00
Sr2	Sr	0.24825	0.02732	0.34723	0.01267	Uiso	1.00
Sr3	Sr	0.00487	0.52964	0.24965	0.01267	Uiso	1.00
Sr4	Sr	0.49512	0.51625	0.43668	0.01267	Uiso	1.00
Sr5	Sr	0.24941	0.02040	0.25099	0.01267	Uiso	1.00
Sr6	Sr	0.25906	0.99835	0.44865	0.01267	Uiso	1.00
Sr7	Sr	0.00450	0.54456	0.34637	0.01267	Uiso	1.00
Sr8	Sr	0.75198	0.02646	0.34655	0.01267	Uiso	1.00
Sr9	Sr	0.50203	0.52524	0.24938	0.01267	Uiso	1.00
Sr10	Sr	0.03166	0.55218	0.44009	0.01267	Uiso	1.00
Sr11	Sr	0.74924	0.02230	0.25029	0.01267	Uiso	1.00
Sr12	Sr	0.74489	0.93508	0.44507	0.01267	Uiso	1.00
Ta1	Ta	0.24848	0.52995	0.30211	0.01267	Uiso	1.00
Ta2	Ta	0.49627	0.02234	0.20843	0.01267	Uiso	1.00
Ta3	Ta	0.49683	0.02321	0.39820	0.01267	Uiso	1.00
Ta4	Ta	0.25515	0.52766	0.20663	0.01267	Uiso	1.00
Ta5	Ta	0.25730	0.53837	0.39159	0.01267	Uiso	1.00
Ta6	Ta	0.00508	0.02257	0.29785	0.01267	Uiso	1.00
Ta7	Ta	0.75139	0.53255	0.30104	0.01267	Uiso	1.00
Ta8	Ta	0.99704	0.02759	0.20840	0.01267	Uiso	1.00
Ta9	Ta	0.99958	0.03972	0.40343	0.01267	Uiso	1.00
Ta10	Ta	0.75632	0.52569	0.20740	0.01267	Uiso	1.00
Ta11	Ta	0.75677	0.52206	0.38918	0.01267	Uiso	1.00
Ta12	Ta	0.50391	0.02088	0.29776	0.01267	Uiso	1.00
Ta13	Ta	0.23036	0.60333	0.52244	0.01267	Uiso	1.00
Ta14	Ta	0.23436	0.87513	0.60261	0.01267	Uiso	1.00
Ta15	Ta	0.23709	0.12724	0.68064	0.01267	Uiso	1.00

Ta16	Ta	0.23929	0.37238	0.75784	0.01267	Uiso	1.00
Ta17	Ta	0.73989	0.06167	0.73251	0.01267	Uiso	1.00
Ta18	Ta	0.72191	0.33611	0.49359	0.01267	Uiso	1.00
Ta19	Ta	0.74308	0.55960	0.57351	0.01267	Uiso	1.00
Ta20	Ta	0.74111	0.80639	0.65268	0.01267	Uiso	1.00
Ta21	Ta	0.53867	0.75147	0.51979	0.01267	Uiso	1.00
Ta22	Ta	0.54475	0.97958	0.59883	0.01267	Uiso	1.00
Ta23	Ta	0.54169	0.23451	0.67615	0.01267	Uiso	1.00
Ta24	Ta	0.55061	0.46279	0.75464	0.01267	Uiso	1.00
Ta25	Ta	0.01425	0.16997	0.49493	0.01267	Uiso	1.00
Ta26	Ta	0.04899	0.45370	0.57690	0.01267	Uiso	1.00
Ta27	Ta	0.04595	0.70450	0.65709	0.01267	Uiso	1.00
Ta28	Ta	0.04414	0.95706	0.73828	0.01267	Uiso	1.00
Ta29	Ta	0.93069	0.69833	0.51821	0.01267	Uiso	1.00
Ta30	Ta	0.93252	0.98430	0.59756	0.01267	Uiso	1.00
Ta31	Ta	0.93525	0.23337	0.67602	0.01267	Uiso	1.00
Ta32	Ta	0.92986	0.46400	0.75475	0.01267	Uiso	1.00
Ta33	Ta	0.42352	0.22835	0.50403	0.01267	Uiso	1.00
Ta34	Ta	0.44023	0.44813	0.58101	0.01267	Uiso	1.00
Ta35	Ta	0.43289	0.70489	0.65784	0.01267	Uiso	1.00
Ta36	Ta	0.43465	0.95537	0.73836	0.01267	Uiso	1.00
O1	O	0.40828	0.34393	0.29668	0.01267	Uiso	1.00
O2	O	0.34784	0.83712	0.29880	0.01267	Uiso	1.00
O3	O	0.10288	0.31216	0.19931	0.01267	Uiso	1.00
O4	O	0.09018	0.33359	0.39126	0.01267	Uiso	1.00
O5	O	0.15907	0.21993	0.29701	0.01267	Uiso	1.00
O6	O	0.14020	0.80526	0.20759	0.01267	Uiso	1.00
O7	O	0.14157	0.83502	0.39311	0.01267	Uiso	1.00
O8	O	0.34934	0.22795	0.20310	0.01267	Uiso	1.00
O9	O	0.34689	0.23031	0.39129	0.01267	Uiso	1.00
O10	O	0.50657	0.04200	0.34204	0.01267	Uiso	1.00
O11	O	0.25707	0.51190	0.24941	0.01267	Uiso	1.00
O12	O	0.25565	0.55220	0.43477	0.01267	Uiso	1.00
O13	O	0.91038	0.34989	0.29805	0.01267	Uiso	1.00
O14	O	0.84614	0.83821	0.29696	0.01267	Uiso	1.00
O15	O	0.60297	0.30681	0.20062	0.01267	Uiso	1.00
O16	O	0.59841	0.32567	0.39060	0.01267	Uiso	1.00
O17	O	0.66080	0.22530	0.29812	0.01267	Uiso	1.00
O18	O	0.63991	0.79914	0.20776	0.01267	Uiso	1.00
O19	O	0.64720	0.80710	0.39682	0.01267	Uiso	1.00
O20	O	0.84856	0.22806	0.20154	0.01267	Uiso	1.00
O21	O	0.84323	0.21519	0.39451	0.01267	Uiso	1.00
O22	O	0.99392	0.02763	0.34224	0.01267	Uiso	1.00
O23	O	0.75784	0.50382	0.25056	0.01267	Uiso	1.00

O24	O	0.72078	0.38228	0.45023	0.01267	Uiso	1.00
N1	N	0.10116	0.72989	0.29542	0.01267	Uiso	1.00
N2	N	0.39137	0.73581	0.19984	0.01267	Uiso	1.00
N3	N	0.39842	0.73709	0.38738	0.01267	Uiso	1.00
N4	N	0.99354	0.04688	0.25078	0.01267	Uiso	1.00
N5	N	0.48630	0.02893	0.43970	0.01267	Uiso	1.00
N6	N	0.24330	0.52208	0.34429	0.01267	Uiso	1.00
N7	N	0.60288	0.72635	0.29626	0.01267	Uiso	1.00
N8	N	0.89111	0.73658	0.20163	0.01267	Uiso	1.00
N9	N	0.89201	0.73469	0.40090	0.01267	Uiso	1.00
N10	N	0.49532	0.03483	0.25118	0.01267	Uiso	1.00
N11	N	0.01660	0.08046	0.44609	0.01267	Uiso	1.00
N12	N	0.75806	0.53685	0.34602	0.01267	Uiso	1.00
N13	N	0.23831	0.15827	0.72533	0.01267	Uiso	1.00
N14	N	0.25918	0.34838	0.49074	0.01267	Uiso	1.00
N15	N	0.22468	0.63885	0.56840	0.01267	Uiso	1.00
N16	N	0.23625	0.87195	0.64869	0.01267	Uiso	1.00
N17	N	0.74174	0.56027	0.52809	0.01267	Uiso	1.00
N18	N	0.74047	0.80794	0.60668	0.01267	Uiso	1.00
N19	N	0.74174	0.05303	0.68663	0.01267	Uiso	1.00
N20	N	0.73890	0.34873	0.76211	0.01267	Uiso	1.00
N21	N	0.10153	0.85773	0.50560	0.01267	Uiso	1.00
N22	N	0.06126	0.40774	0.53101	0.01267	Uiso	1.00
N23	N	0.06333	0.68426	0.61228	0.01267	Uiso	1.00
N24	N	0.06337	0.93897	0.69204	0.01267	Uiso	1.00
N25	N	0.10569	0.13597	0.59125	0.01267	Uiso	1.00
N26	N	0.10671	0.38403	0.66884	0.01267	Uiso	1.00
N27	N	0.11088	0.65381	0.74987	0.01267	Uiso	1.00
N28	N	0.06583	0.22735	0.77052	0.01267	Uiso	1.00
N29	N	0.56681	0.99367	0.64336	0.01267	Uiso	1.00
N30	N	0.56191	0.27405	0.72024	0.01267	Uiso	1.00
N31	N	0.61022	0.04553	0.50412	0.01267	Uiso	1.00
N32	N	0.60821	0.29950	0.58604	0.01267	Uiso	1.00
N33	N	0.60584	0.54926	0.66336	0.01267	Uiso	1.00
N34	N	0.60547	0.81934	0.74465	0.01267	Uiso	1.00
N35	N	0.54819	0.49132	0.48929	0.01267	Uiso	1.00
N36	N	0.56517	0.74924	0.56457	0.01267	Uiso	1.00
N37	N	0.36746	0.87538	0.51173	0.01267	Uiso	1.00
N38	N	0.40313	0.42627	0.53789	0.01267	Uiso	1.00
N39	N	0.40913	0.69251	0.61274	0.01267	Uiso	1.00
N40	N	0.41214	0.93679	0.69212	0.01267	Uiso	1.00
N41	N	0.37211	0.13707	0.59336	0.01267	Uiso	1.00
N42	N	0.37141	0.38344	0.66912	0.01267	Uiso	1.00
N43	N	0.36750	0.65422	0.75027	0.01267	Uiso	1.00

N44	N	0.41327	0.22663	0.77023	0.01267	Uiso	1.00
N45	N	0.91313	0.99887	0.64248	0.01267	Uiso	1.00
N46	N	0.91770	0.27643	0.72041	0.01267	Uiso	1.00
N47	N	0.85860	0.02216	0.50302	0.01267	Uiso	1.00
N48	N	0.87109	0.29774	0.58406	0.01267	Uiso	1.00
N49	N	0.87209	0.55080	0.66349	0.01267	Uiso	1.00
N50	N	0.87352	0.82095	0.74506	0.01267	Uiso	1.00
N51	N	0.90816	0.47468	0.48477	0.01267	Uiso	1.00
N52	N	0.91640	0.74470	0.56351	0.01267	Uiso	1.00

The structural information of Ta₃N₅/Ta₂O₃N:

_cell_length_a				10.7926			
_cell_length_b				5.5644			
_cell_length_c				44.9113			
_cell_angle_alpha				90.0000			
_cell_angle_beta				90.0000			
_cell_angle_gamma				90.0000			
loop_							
_atom_site_label							
_atom_site_type_symbol							
_atom_site_fract_x							
_atom_site_fract_y							
_atom_site_fract_z							
_atom_site_U_iso_or_equiv							
_atom_site_adp_type							
_atom_site_occupancy							
Sr1	Sr	0.53579	0.49879	0.29588	0.01267	Uiso	1.00
Sr2	Sr	0.27883	0.99562	0.29381	0.01267	Uiso	1.00
Sr3	Sr	0.02219	0.49627	0.20303	0.01267	Uiso	1.00
Sr4	Sr	0.53288	0.49451	0.39327	0.01267	Uiso	1.00
Sr5	Sr	0.28116	0.99922	0.20109	0.01267	Uiso	1.00
Sr6	Sr	0.29118	0.95613	0.39186	0.01267	Uiso	1.00
Sr7	Sr	0.02833	0.50131	0.29595	0.01267	Uiso	1.00
Sr8	Sr	0.78180	0.99731	0.29674	0.01267	Uiso	1.00
Sr9	Sr	0.54017	0.49585	0.20240	0.01267	Uiso	1.00
Sr10	Sr	0.03689	0.48634	0.38967	0.01267	Uiso	1.00
Sr11	Sr	0.78304	0.99778	0.20322	0.01267	Uiso	1.00
Sr12	Sr	0.77750	-0.02327	0.38879	0.01267	Uiso	1.00
Ta1	Ta	0.27884	0.50541	0.24698	0.01267	Uiso	1.00
Ta2	Ta	0.27539	0.51132	0.44592	0.01267	Uiso	1.00
Ta3	Ta	0.52204	0.98874	0.34344	0.01267	Uiso	1.00
Ta4	Ta	0.28478	0.49490	0.33658	0.01267	Uiso	1.00

Ta5	Ta	0.03423	0.99536	0.24354	0.01267	Uiso	1.00
Ta6	Ta	0.02961	0.98584	0.42995	0.01267	Uiso	1.00
Ta7	Ta	0.77687	0.50424	0.25157	0.01267	Uiso	1.00
Ta8	Ta	0.79243	0.50036	0.44042	0.01267	Uiso	1.00
Ta9	Ta	0.03240	0.98999	0.34345	0.01267	Uiso	1.00
Ta10	Ta	0.78148	0.49683	0.34274	0.01267	Uiso	1.00
Ta11	Ta	0.53345	0.99558	0.24248	0.01267	Uiso	1.00
Ta12	Ta	0.54147	0.98281	0.43671	0.01267	Uiso	1.00
Ta13	Ta	0.21013	0.66903	0.52495	0.01267	Uiso	1.00
Ta14	Ta	0.20623	0.90277	0.60429	0.01267	Uiso	1.00
Ta15	Ta	0.20910	0.15431	0.68235	0.01267	Uiso	1.00
Ta16	Ta	0.21051	0.39988	0.75960	0.01267	Uiso	1.00
Ta17	Ta	0.71082	0.08893	0.73418	0.01267	Uiso	1.00
Ta18	Ta	0.68394	0.33375	0.49877	0.01267	Uiso	1.00
Ta19	Ta	0.71424	0.58071	0.57657	0.01267	Uiso	1.00
Ta20	Ta	0.71336	0.83337	0.65454	0.01267	Uiso	1.00
Ta21	Ta	0.50622	0.75700	0.52339	0.01267	Uiso	1.00
Ta22	Ta	0.51448	0.00625	0.60075	0.01267	Uiso	1.00
Ta23	Ta	0.51336	0.26040	0.67786	0.01267	Uiso	1.00
Ta24	Ta	0.52165	0.49013	0.75630	0.01267	Uiso	1.00
Ta25	Ta	0.00481	0.21180	0.49992	0.01267	Uiso	1.00
Ta26	Ta	0.02038	0.48267	0.57833	0.01267	Uiso	1.00
Ta27	Ta	0.01771	0.73390	0.65872	0.01267	Uiso	1.00
Ta28	Ta	0.01509	0.98438	0.74006	0.01267	Uiso	1.00
Ta29	Ta	0.89160	0.74130	0.51911	0.01267	Uiso	1.00
Ta30	Ta	0.90379	0.00982	0.59920	0.01267	Uiso	1.00
Ta31	Ta	0.90783	0.26195	0.67774	0.01267	Uiso	1.00
Ta32	Ta	0.90101	0.49130	0.75646	0.01267	Uiso	1.00
Ta33	Ta	0.39924	0.24739	0.50156	0.01267	Uiso	1.00
Ta34	Ta	0.40792	0.47285	0.58158	0.01267	Uiso	1.00
Ta35	Ta	0.40498	0.72976	0.65925	0.01267	Uiso	1.00
Ta36	Ta	0.40531	0.98274	0.73999	0.01267	Uiso	1.00
O1	O	0.44246	0.30931	0.24925	0.01267	Uiso	1.00
O2	O	0.39984	0.18980	0.45678	0.01267	Uiso	1.00
O3	O	0.37622	0.81273	0.24720	0.01267	Uiso	1.00
O4	O	0.41135	0.71699	0.43598	0.01267	Uiso	1.00
O5	O	0.12673	0.32252	0.34222	0.01267	Uiso	1.00
O6	O	0.19161	0.18928	0.24764	0.01267	Uiso	1.00
O7	O	0.07864	0.22901	0.46006	0.01267	Uiso	1.00
O8	O	0.18561	0.79589	0.34205	0.01267	Uiso	1.00
O9	O	0.36883	0.18814	0.34547	0.01267	Uiso	1.00
O10	O	0.51863	0.99287	0.29977	0.01267	Uiso	1.00
O11	O	0.28929	0.48969	0.20241	0.01267	Uiso	1.00
O12	O	0.26122	0.37353	0.40684	0.01267	Uiso	1.00

O13	O	0.94117	0.30736	0.24967	0.01267	Uiso	1.00
O14	O	0.88908	0.22971	0.42461	0.01267	Uiso	1.00
O15	O	0.87861	0.80879	0.24967	0.01267	Uiso	1.00
O16	O	0.91157	0.73533	0.42570	0.01267	Uiso	1.00
O17	O	0.62074	0.29919	0.34279	0.01267	Uiso	1.00
O18	O	0.68883	0.18662	0.24951	0.01267	Uiso	1.00
O19	O	0.66293	0.24749	0.45161	0.01267	Uiso	1.00
O20	O	0.67691	0.80239	0.34228	0.01267	Uiso	1.00
O21	O	0.87899	0.19636	0.34424	0.01267	Uiso	1.00
O22	O	0.03549	0.01059	0.29816	0.01267	Uiso	1.00
O23	O	0.78619	0.48707	0.20397	0.01267	Uiso	1.00
O24	O	0.76049	0.48845	0.38750	0.01267	Uiso	1.00
N1	N	0.13047	0.69297	0.24900	0.01267	Uiso	1.00
N2	N	0.15968	0.75815	0.43882	0.01267	Uiso	1.00
N3	N	0.42494	0.69585	0.35049	0.01267	Uiso	1.00
N4	N	0.03073	0.99898	0.20126	0.01267	Uiso	1.00
N5	N	0.53435	0.03570	0.39490	0.01267	Uiso	1.00
N6	N	0.29216	0.49660	0.29475	0.01267	Uiso	1.00
N7	N	0.62870	0.69588	0.24915	0.01267	Uiso	1.00
N8	N	0.66399	0.74152	0.43633	0.01267	Uiso	1.00
N9	N	0.92790	0.70772	0.34525	0.01267	Uiso	1.00
N10	N	0.53360	0.00128	0.20039	0.01267	Uiso	1.00
N11	N	0.05957	0.02008	0.38831	0.01267	Uiso	1.00
N12	N	0.78182	0.49043	0.29668	0.01267	Uiso	1.00
N13	N	0.20967	0.18609	0.72707	0.01267	Uiso	1.00
N14	N	0.24479	0.44985	0.49080	0.01267	Uiso	1.00
N15	N	0.19975	0.65553	0.57105	0.01267	Uiso	1.00
N16	N	0.20541	0.90017	0.65013	0.01267	Uiso	1.00
N17	N	0.71540	0.56629	0.53169	0.01267	Uiso	1.00
N18	N	0.71434	0.83720	0.60894	0.01267	Uiso	1.00
N19	N	0.71223	0.08149	0.68843	0.01267	Uiso	1.00
N20	N	0.70979	0.37647	0.76387	0.01267	Uiso	1.00
N21	N	0.07169	0.90855	0.51360	0.01267	Uiso	1.00
N22	N	0.02973	0.45669	0.53178	0.01267	Uiso	1.00
N23	N	0.03202	0.71235	0.61353	0.01267	Uiso	1.00
N24	N	0.03522	0.96568	0.69392	0.01267	Uiso	1.00
N25	N	0.07764	0.16286	0.59189	0.01267	Uiso	1.00
N26	N	0.07834	0.41217	0.67052	0.01267	Uiso	1.00
N27	N	0.08175	0.68136	0.75181	0.01267	Uiso	1.00
N28	N	0.03689	0.25462	0.77237	0.01267	Uiso	1.00
N29	N	0.53788	0.01991	0.64512	0.01267	Uiso	1.00
N30	N	0.53250	0.30059	0.72201	0.01267	Uiso	1.00
N31	N	0.57502	0.06203	0.50907	0.01267	Uiso	1.00
N32	N	0.57790	0.32304	0.58794	0.01267	Uiso	1.00

N33	N	0.57715	0.57560	0.66504	0.01267	Uiso	1.00
N34	N	0.57624	0.84650	0.74632	0.01267	Uiso	1.00
N35	N	0.53105	0.51914	0.49111	0.01267	Uiso	1.00
N36	N	0.53908	0.77004	0.56740	0.01267	Uiso	1.00
N37	N	0.33959	0.92162	0.51641	0.01267	Uiso	1.00
N38	N	0.38016	0.45862	0.53805	0.01267	Uiso	1.00
N39	N	0.37971	0.71619	0.61442	0.01267	Uiso	1.00
N40	N	0.38260	0.96292	0.69370	0.01267	Uiso	1.00
N41	N	0.34228	0.16026	0.59445	0.01267	Uiso	1.00
N42	N	0.34275	0.40965	0.67079	0.01267	Uiso	1.00
N43	N	0.33832	0.68177	0.75202	0.01267	Uiso	1.00
N44	N	0.38422	0.25400	0.77207	0.01267	Uiso	1.00
N45	N	0.88595	0.02634	0.64444	0.01267	Uiso	1.00
N46	N	0.88901	0.30338	0.72217	0.01267	Uiso	1.00
N47	N	0.84097	0.06031	0.50441	0.01267	Uiso	1.00
N48	N	0.84430	0.32840	0.58693	0.01267	Uiso	1.00
N49	N	0.84355	0.57847	0.66533	0.01267	Uiso	1.00
N50	N	0.84447	0.84817	0.74675	0.01267	Uiso	1.00
N51	N	0.85140	0.52080	0.48216	0.01267	Uiso	1.00
N52	N	0.88491	0.77817	0.56448	0.01267	Uiso	1.00