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## **Supporting Materials**

## Insight into Enhanced Photocatalytic Activity of SrTiO<sub>3</sub> in Presence of (Ni,

## V/Nb/Ta/Sb) Pair

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**Fig. S1:** Variation of defect formation energy with the host chemical potential for the doping of Ni/V/Nb/Ta/Sb into (a) Sr lattice site of SrTiO<sub>3</sub> and (b) interstitial site of SrTiO<sub>3</sub>.

## Table S1: Details of bond length for 1:1 and 1:2 type codoped systems using $2 \times 2 \times 2$ supercell

System	d <sub>M-M</sub>	d <sub>M-O</sub>	d <sub>Ni-M</sub>	d <sub>Ni-O</sub> (Å)
	(M=V/Nb/Ta/Sb)	(M=V/Nb/Ta/S	(M=V/Nb/Ta/Sb)	
	(Å)	b) (Å)	(Å)	
(Ni, V)-SrTiO <sub>3</sub>		1.861, 1.915	3.942	1.948, 2.081
(Ni, Nb)-SrTiO <sub>3</sub>		1.985, 1.994	3.947	1.962, 1.200
(Ni, Ta)-SrTiO <sub>3</sub>		1.973, 1.982	3.948	1.975, 1.995
(Ni, Sb)-SrTiO <sub>3</sub>		1.958, 1.982	3.972	2.014, 1.972
(Ni, 2V)-SrTiO <sub>3</sub>	5.55	1.85, 1.934		1.995, 2.076
(Ni, 2Nb)-	3.993	1.961-2.009		2.023-2.074
SrTiO <sub>3</sub>				
(Ni, 2Ta)-	5.624	1.947, 2.004		2.029, 2.068
SrTiO <sub>3</sub>				
(Ni, 2Sb)-	5.630	1.943, 2.008		2.038, 2.054
SrTiO <sub>3</sub>				



**Fig. S2:** Density of states of (a) (Ni, 2V)-codoped  $SrTiO_3$ , (b) (Ni, 2Nb)-doped  $SrTiO_3$ , (c) (Ni, 2Ta)-doped  $SrTiO_3$  and (d) (Ni, 2Sb)-doped  $SrTiO_3$  using  $2 \times 2 \times 3$  supercell. Vertical dashed line indicates Fermi Level.



**Fig. S3:** Density of states of (a) (Ni, 2V)-codoped  $SrTiO_3$ , (b) (Ni, 2Nb)-doped  $SrTiO_3$ , (c) (Ni, 2Ta)-doped  $SrTiO_3$  and (d) (Ni, 2Sb)-doped  $SrTiO_3$  using  $2 \times 3 \times 3$  supercell. Vertical dashed line indicates Fermi Level.

Systems	Concentration		d <sub>M-M</sub>	d <sub>M-O</sub>	d <sub>Ni-O</sub> (Å)	Band Gap
	Ni	М	(M=V/Nb/T	(M=V/Nb/T		(eV)
	(%)	(M=V/Nb/Ta /Sb) (%)	a/Sb) (Å)	a/Sb) (Å)		
(Ni, 2V)-	8.33	16.67	5.476	1.778-2.145	2.003-2.089	1.98
SrTiO <sub>3</sub>	5.55	11.11	4.018	1.747-2.275	2.036-2.107	2.46
(Ni, 2Nb)	8.33	16.67	5.592	1.950-2.067	2.01-2.054	2.42
-SrTiO <sub>3</sub>	5.55	11.11	5.569	1.940-2.059	2.019-2.043	2.97
(Ni, 2Ta)	8.33	16.67	5.605	1.949-1.997	2.018-2.056	2.55
-SrTiO <sub>3</sub>	5.55	11.11	5.587	1.935-2.023	2.029-2.042	2.67
(Ni, 2Sb)	8.33	16.67	5.63	1.943-2.013	2.023-2.08	2.88
-SrTiO <sub>3</sub>	5.55	11.11	5.626	1.951-2.003	2.016-2.067	2.92

Table S2: Details of structural parameter and band gap for 1:2 type codoped systems using  $2 \times 2 \times 3$  supercell and  $2 \times 3 \times 3$  supercell.