Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Materials

Insight into Enhanced Photocatalytic Activity of $SrTiO_3$ in Presence of (Ni, V/Nb/Ta/Sb) Pair

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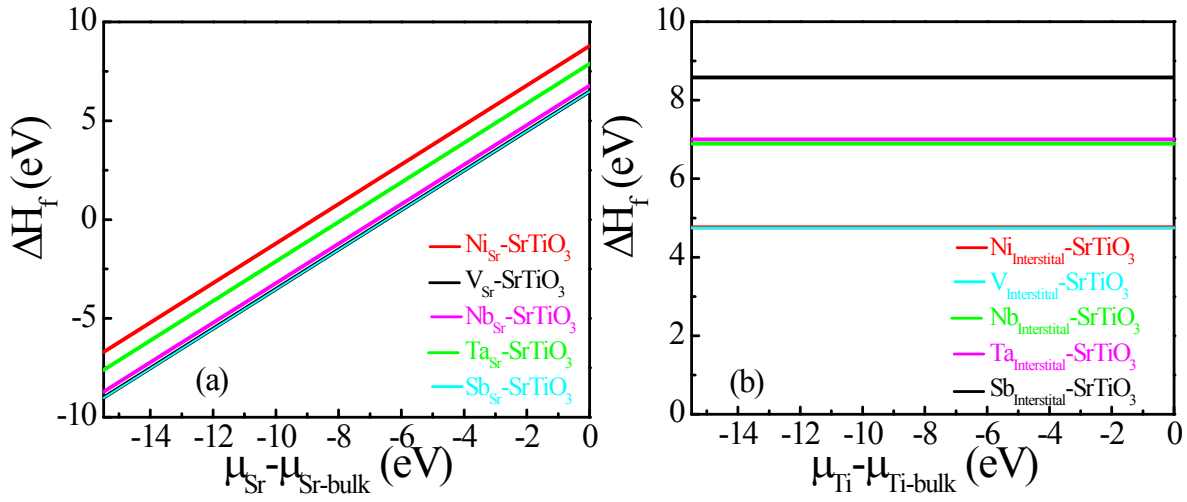

Fig. S1: Variation of defect formation energy with the host chemical potential for the doping of Ni/V/Nb/Ta/Sb into (a) Sr lattice site of $SrTiO_3$ and (b) interstitial site of $SrTiO_3$.

Table S1: Details of bond length for 1:1 and 1:2 type codoped systems using 2 × 2 × 2 supercell

System	d_{M-M} (M=V/Nb/Ta/Sb) **(Å)**	d_{M-O} (M=V/Nb/Ta/Sb) **(Å)**	d_{Ni-M} (M=V/Nb/Ta/Sb) **(Å)**	d_{Ni-O} **(Å)**
(Ni, V)-$SrTiO_3$		1.861, 1.915	3.942	1.948, 2.081
(Ni, Nb)-$SrTiO_3$		1.985, 1.994	3.947	1.962, 1.200
(Ni, Ta)-$SrTiO_3$		1.973, 1.982	3.948	1.975, 1.995
(Ni, Sb)-$SrTiO_3$		1.958, 1.982	3.972	2.014, 1.972
(Ni, 2V)-$SrTiO_3$	5.55	1.85, 1.934		1.995, 2.076
(Ni, 2Nb)-$SrTiO_3$	3.993	1.961-2.009		2.023-2.074
(Ni, 2Ta)-$SrTiO_3$	5.624	1.947, 2.004		2.029, 2.068
(Ni, 2Sb)-$SrTiO_3$	5.630	1.943, 2.008		2.038, 2.054

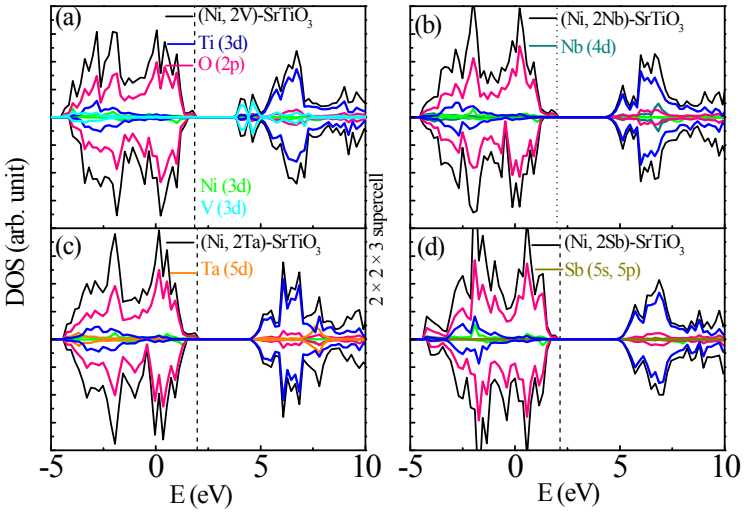

Fig. S2: Density of states of (a) (Ni, 2V)-codoped $SrTiO_3$, (b) (Ni, 2Nb)-doped $SrTiO_3$, (c) (Ni, 2Ta)-doped $SrTiO_3$ and (d) (Ni, 2Sb)-doped $SrTiO_3$ using 2 × 2 × 3 supercell. Vertical dashed line indicates Fermi Level.

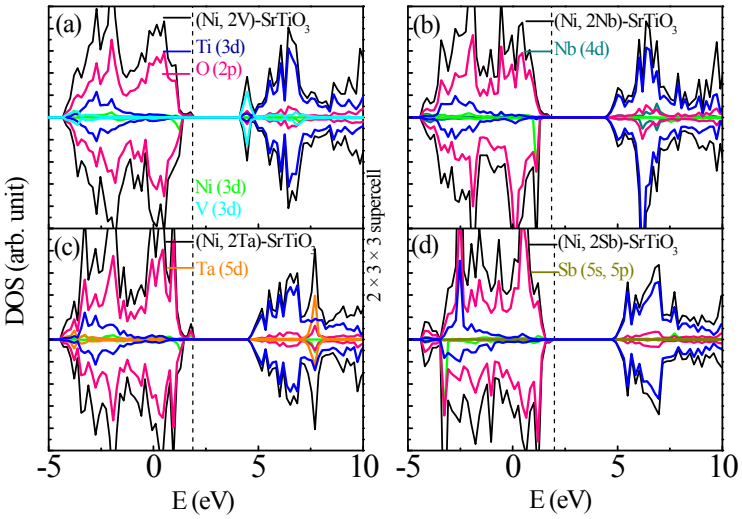

Fig. S3: Density of states of (a) (Ni, 2V)-codoped $SrTiO_3$, (b) (Ni, 2Nb)-doped $SrTiO_3$, (c) (Ni, 2Ta)-doped $SrTiO_3$ and (d) (Ni, 2Sb)-doped $SrTiO_3$ using 2 × 3 × 3 supercell. Vertical dashed line indicates Fermi Level.

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

Systems	Concentration		d_{M-M} (M=V/Nb/Ta/Sb) **(Å)**	d_{M-O} (M=V/Nb/Ta/Sb) **(Å)**	d_{Ni-O} **(Å)**	Band Gap (eV)
	Ni (%)	M (M=V/Nb/Ta/Sb) (%)				
(Ni, 2V)-$SrTiO_3$	8.33	16.67	5.476	1.778-2.145	2.003-2.089	1.98
	5.55	11.11	4.018	1.747-2.275	2.036-2.107	2.46
(Ni, 2Nb)-$SrTiO_3$	8.33	16.67	5.592	1.950-2.067	2.01-2.054	2.42
	5.55	11.11	5.569	1.940-2.059	2.019-2.043	2.97
(Ni, 2Ta)-$SrTiO_3$	8.33	16.67	5.605	1.949-1.997	2.018-2.056	2.55
	5.55	11.11	5.587	1.935-2.023	2.029-2.042	2.67
(Ni, 2Sb)-$SrTiO_3$	8.33	16.67	5.63	1.943-2.013	2.023-2.08	2.88
	5.55	11.11	5.626	1.951-2.003	2.016-2.067	2.92