Supporting Information

Rational Selection of Transition Metal Co-dopant in Sulfur-doped Titanium Dioxide

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Table S1. Effect of various transition metals on the properties of TM-doped titanium dioxide.

Dopant	Lattice Parameters			Volume	Total Energy	Density	Relative Volume Difference	Relative Energy Difference	Relative Density Difference
	a	b	c						
	Å	Å	Å	Å^3	kcal/mol	g/cm^3	Å^3	kcal/mol	g/cm^3
Sc	7.575	7.569	8.618	494.069	2471.883	4.287	99.8805	105.2505	99.8891
Ti	7.623	7.623	8.512	494.660	2348.571	4.291	100.0000	100.0000	100.0000
V	7.538	7.546	8.606	489.449	2516.600	4.347	98.9466	107.1545	101.3051
Cr	7.620	7.620	8.484	492.641	2348.918	4.323	99.5918	100.0148	100.7365
Mn	7.662	7.662	8.474	497.477	2341.802	4.291	100.5694	99.7118	99.9812
Fe	7.625	7.626	8.485	493.325	2342.563	4.330	99.7302	99.7442	100.8939
Co	7.606	7.605	8.466	489.734	2369.146	4.372	99.0041	100.8761	101.8776
Ni	7.587	7.586	8.453	486.446	2398.315	4.401	98.3395	102.1181	102.5484
Cu	7.569	7.573	8.534	489.119	2489.472	4.393	98.8799	105.9994	102.3706
Zn	7.583	7.582	8.501	488.703	2478.755	4.403	98.7958	105.5431	102.6029

Table S2. Effect of various transition metals on the properties of TM/S co-doped titanium dioxide.

Dopant	Lattice Parameters			Volume	Total Energy	Density	Relative Volume Difference	Relative Energy Difference	Relative Density Difference
	a	b	c						
	Å	Å	Å	Å^3	kcal/mol	g/cm^3	Å^3	kcal/mol	g/cm^3
Sc	7.588	7.651	8.720	506.239	2493.499	4.2363	100.4410	104.8460	99.3345
Ti	7.614	7.685	8.615	504.016	2378.248	4.2646	100.0000	100.0000	100.0000
V	7.557	7.618	8.711	501.372	2530.647	4.2972	99.4753	106.4080	100.7637
Cr	7.606	7.677	8.587	501.389	2376.402	4.3006	99.4788	99.9224	100.8421
Mn	7.617	7.689	8.592	503.145	2366.379	4.2953	99.8271	99.5009	100.7178
Fe	7.611	7.683	8.587	502.143	2370.736	4.3068	99.6283	99.6841	100.9893
Co	7.587	7.659	8.569	497.923	2393.718	4.3536	98.7911	100.6505	102.0865
Ni	7.565	7.637	8.554	494.145	2419.922	4.3862	98.0416	101.7523	102.8494
Cu	7.584	7.644	8.633	500.476	2499.966	4.3467	99.2976	105.1180	101.9246
Zn	7.595	7.655	8.594	499.655	2487.881	4.3600	99.1347	104.6098	102.2350

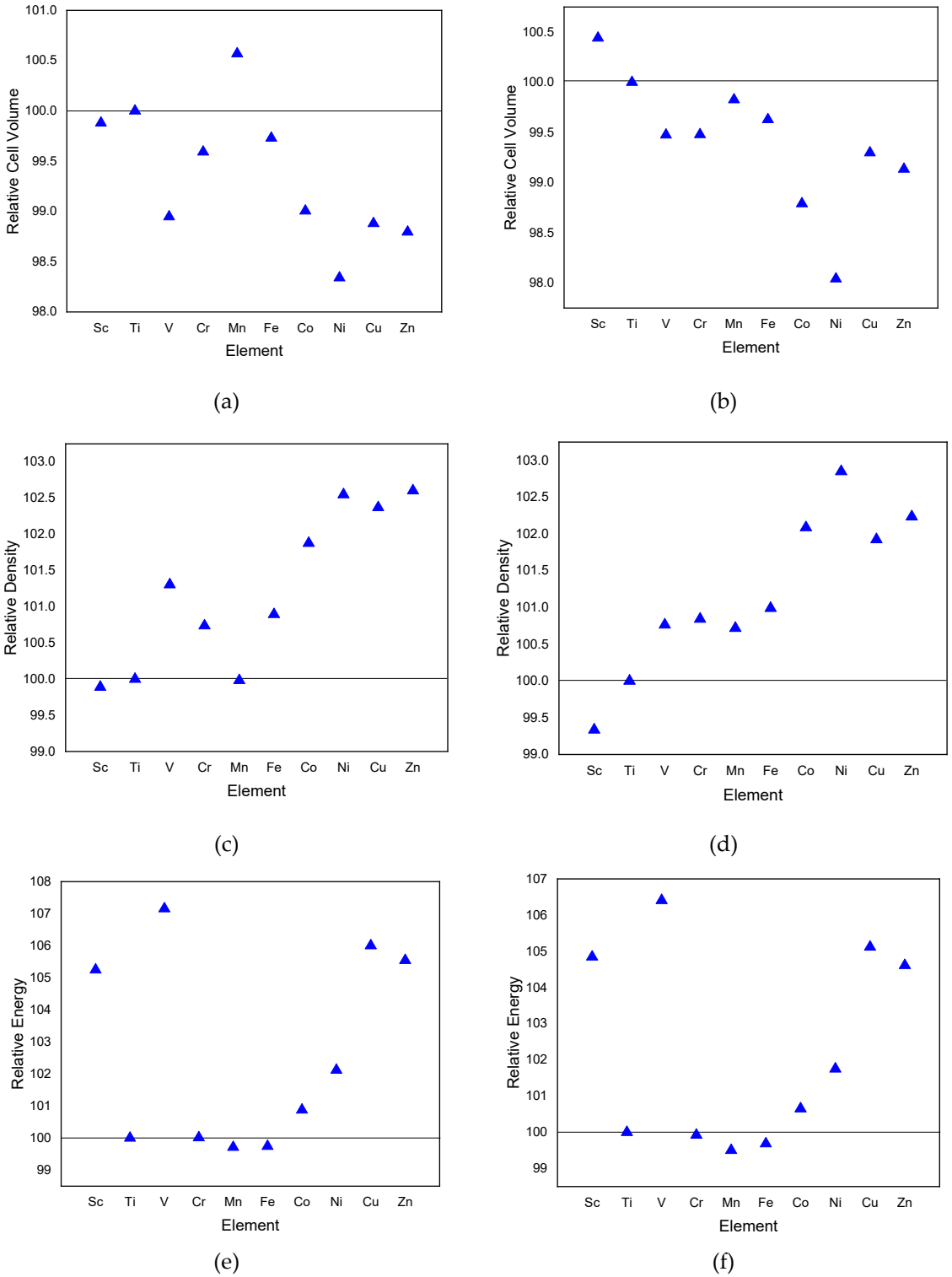

Figure S1 Calculated cell volume differences of (a) TM-doped TiO_2 relative to pristine TiO_2 and (b) TM/S co-doped TiO_2 relative to S-doped TiO_2; Calculated density differences of (c) TM-doped TiO_2 relative to pristine TiO_2 and (d) TM/S co-doped TiO_2 relative to S-doped TiO_2; and Calculated energy differences of (e) TM-doped TiO_2 relative to pristine TiO_2 and (f) TM/S co-doped TiO_2 relative to S-doped TiO_2.

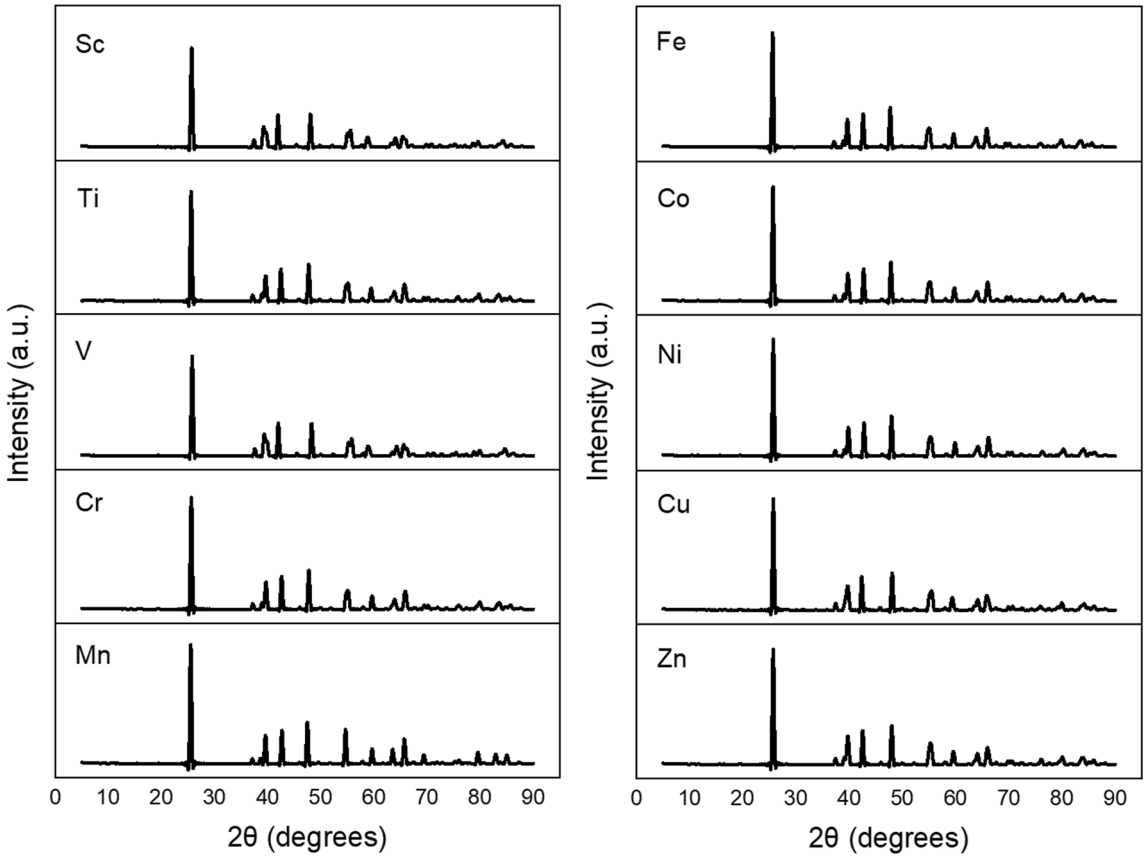

Figure S2. Simulated XRD profiles of various TM-doped TiO_2.

Table S3. Effect of various transition metals on the crystallinity of TM-doped titanium dioxide.

Co-dopant	Degree of Crystallinity	Relative Difference vs. S-TiO_2
Sc	64.14	117.93
Ti	54.39	100.00
V	65.13	119.75
Cr	54.14	99.54
Mn	55.02	101.16
Fe	53.54	98.44
Co	54.13	99.52
Ni	53.62	98.58
Cu	56.25	103.42
Zn	54.76	100.68

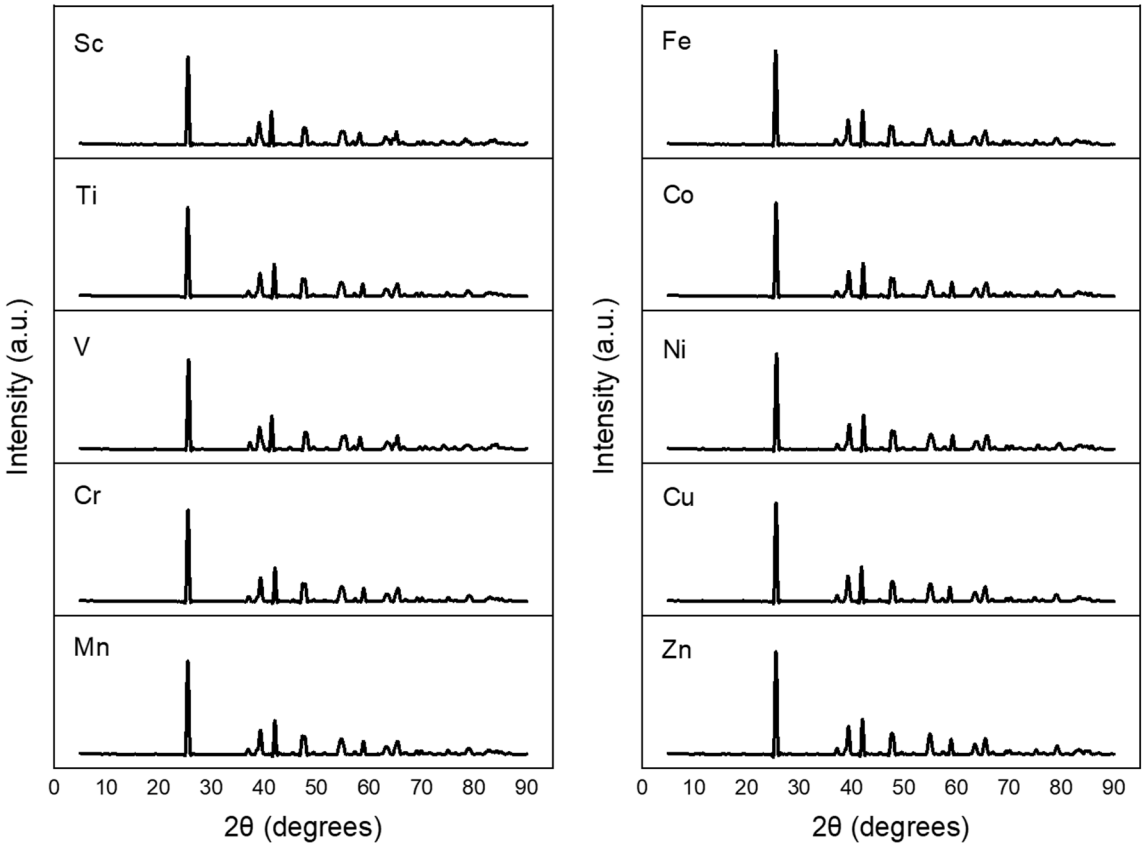

Figure S3. Simulated XRD profiles of various TM/S co-doped TiO_2.

Table S4. Effect of various transition metals on the crystallinity of TM/S co-doped titanium dioxide.

Co-dopant	Degree of Crystallinity	Relative Difference vs. S-TiO_2
Sc	62.43	99.05
Ti	63.03	100.00
V	64.16	101.79
Cr	64.08	101.67
Mn	63.35	100.51
Fe	63.39	100.57
Co	64.13	101.75
Ni	64.92	103.00
Cu	64.85	102.89
Zn	66.56	105.60

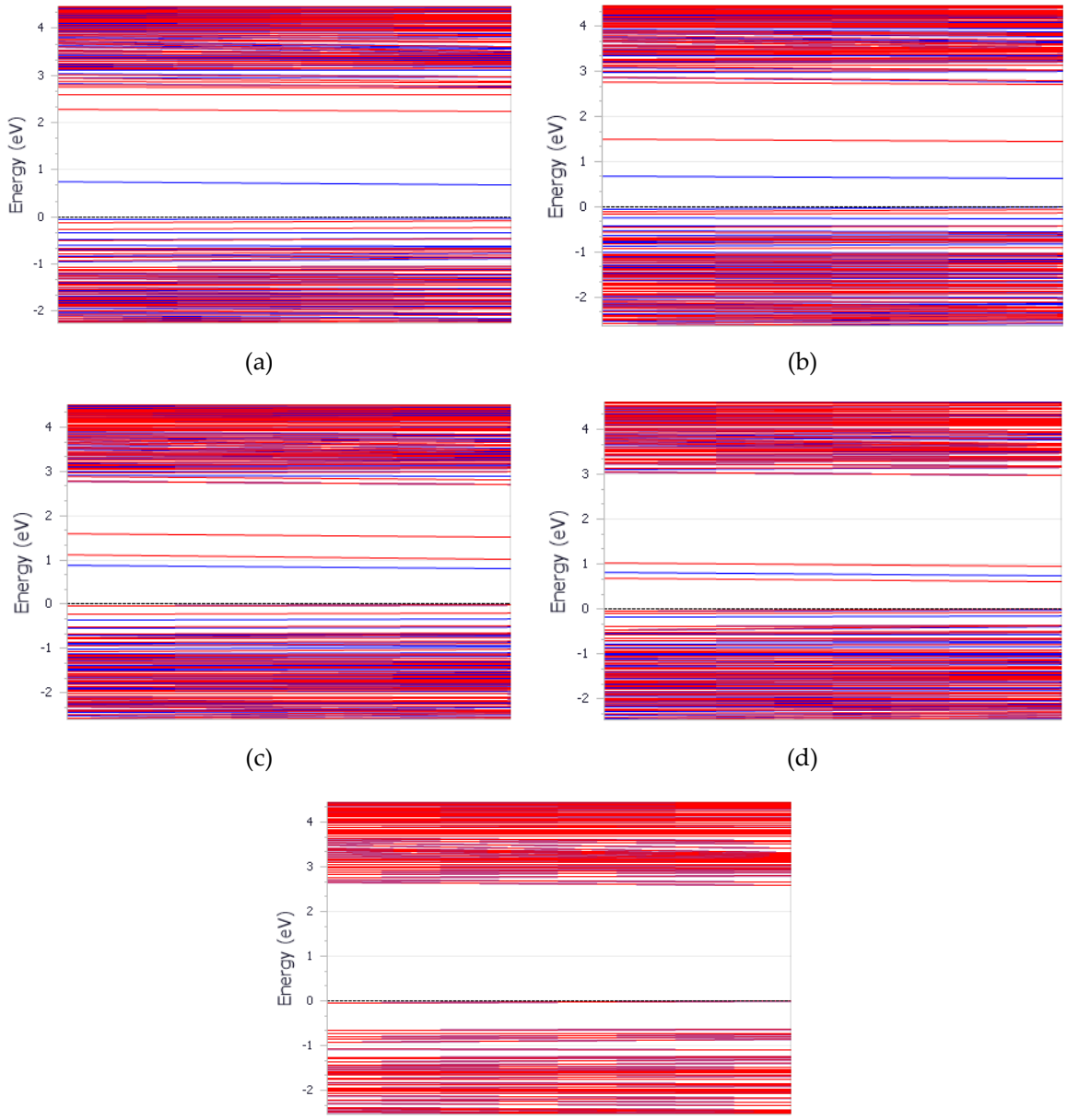

Figure S4. Electronic structure of: (a) Fe/S–TiO_2, (b) Co/S–TiO_2, (c) Ni/S–TiO_2, (d) Cu/S–TiO_2, and (e) S–TiO_2.

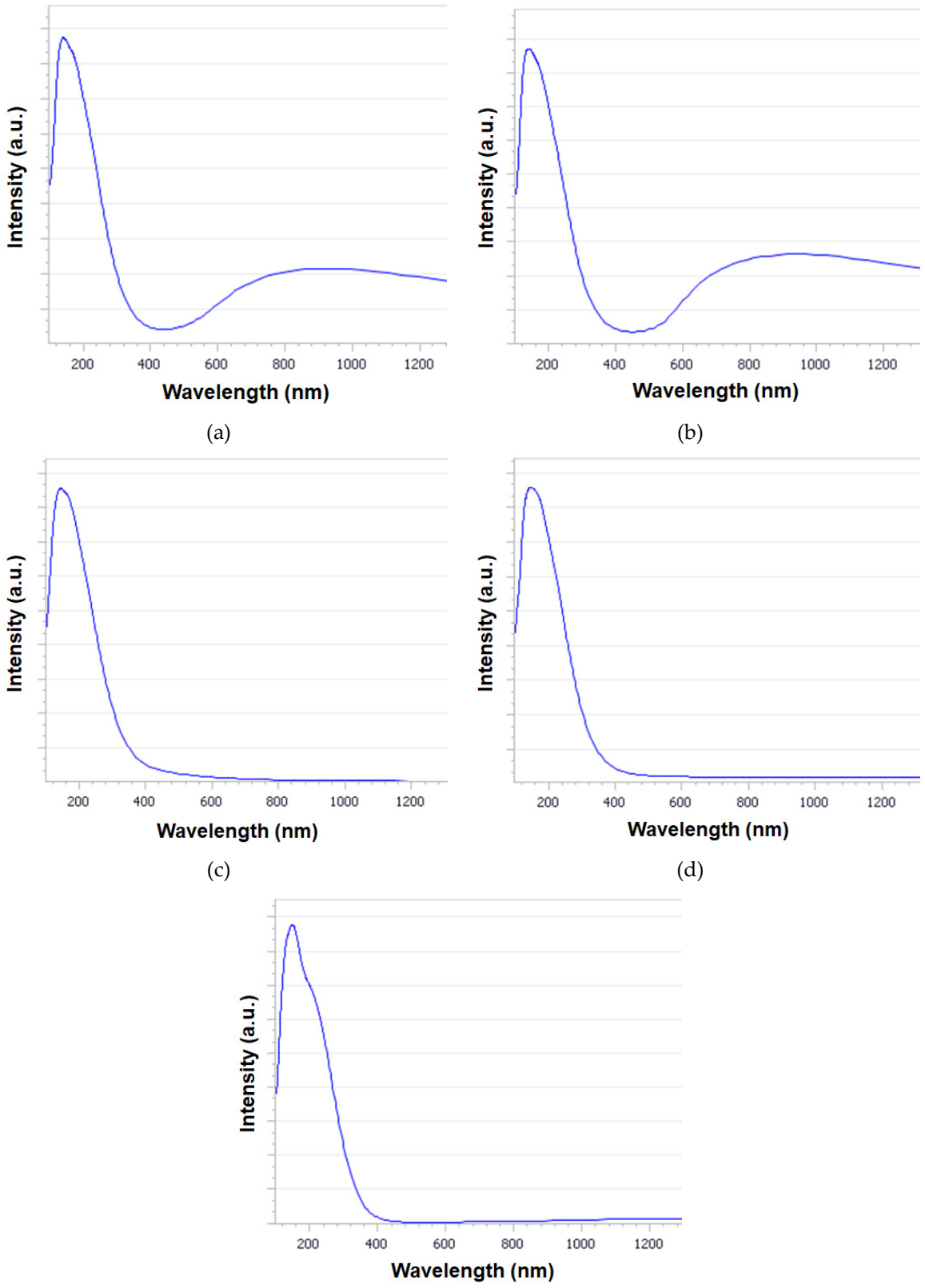

Figure S5. Optical absorption spectra of: (a) Fe/S–TiO_2, (b) Co/S–TiO_2, (c) Ni/S–TiO_2, (d) Cu/S–TiO_2, and (e) pristine TiO_2.

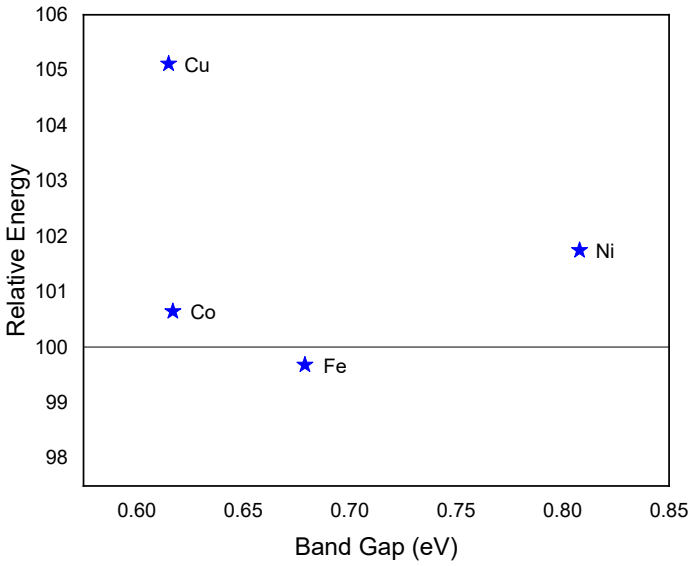

Figure S6. Volcano plot of late transition metals and sulfur co-doped TiO_2.