Supporting information

Classifying oxide states in XAS spectra using machine learning

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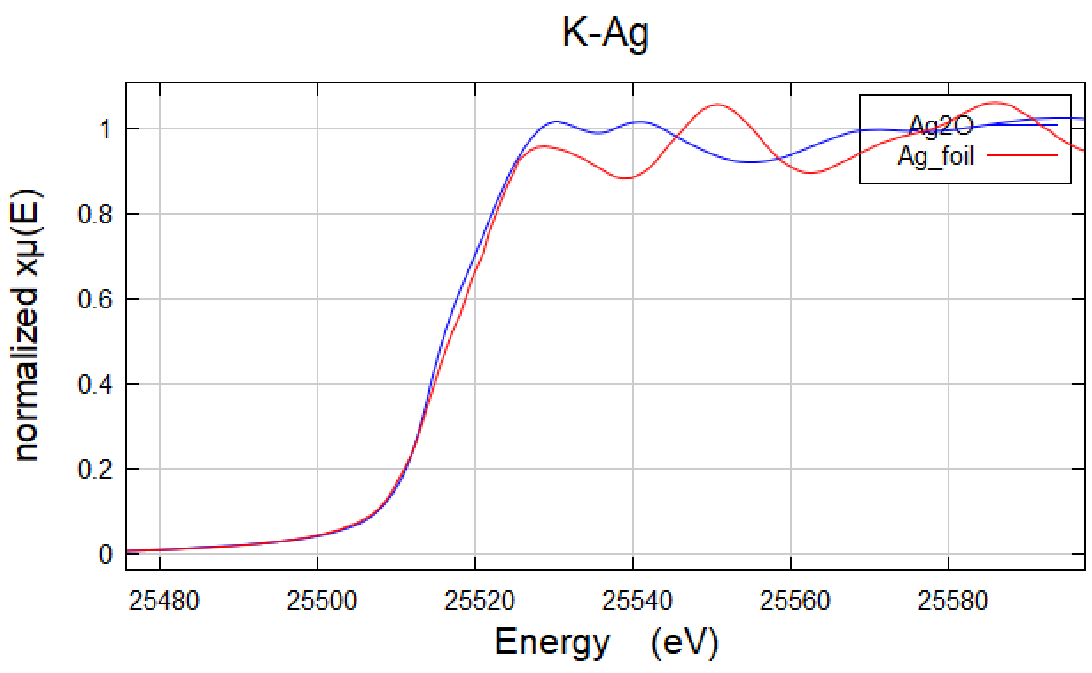

Figure S- 1 Source XANES Spectra for data mining (Ag-K edg)e

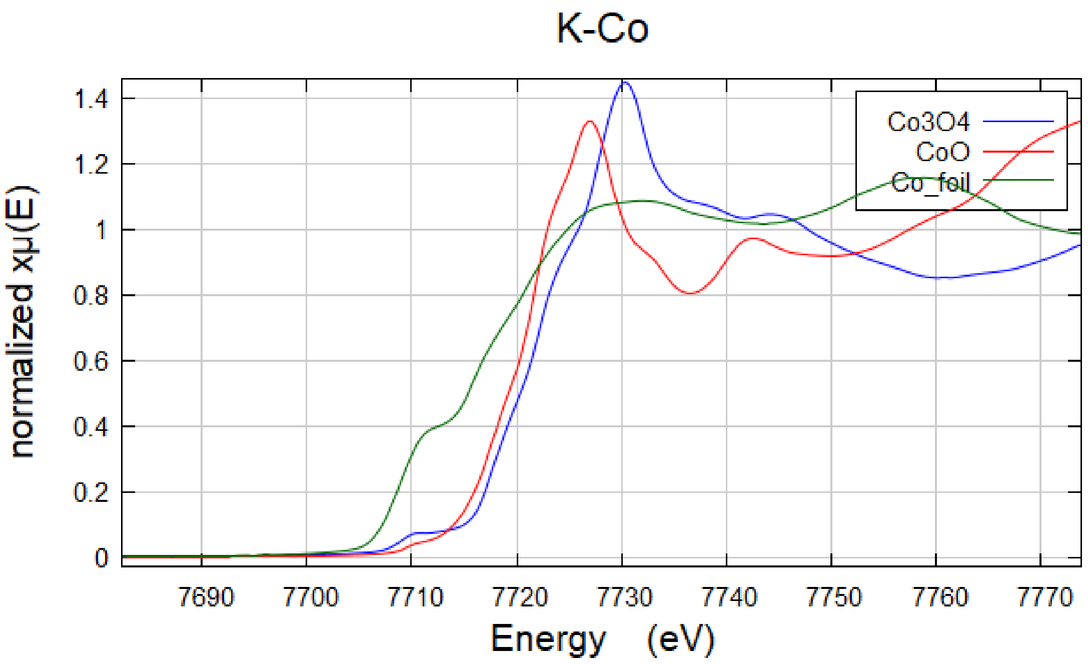

Figure S- 2 **Analyzed XANES Spectra of Co-K edge**

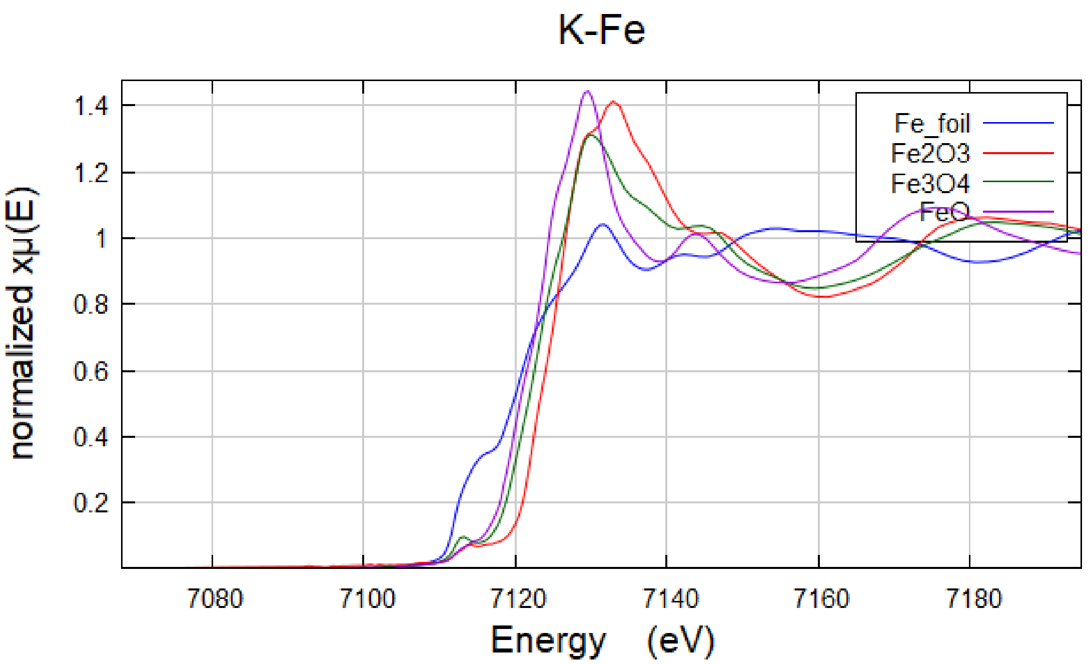

Figure S- 3 **Source XANES Spectra for data mining (Fe-K edge)**

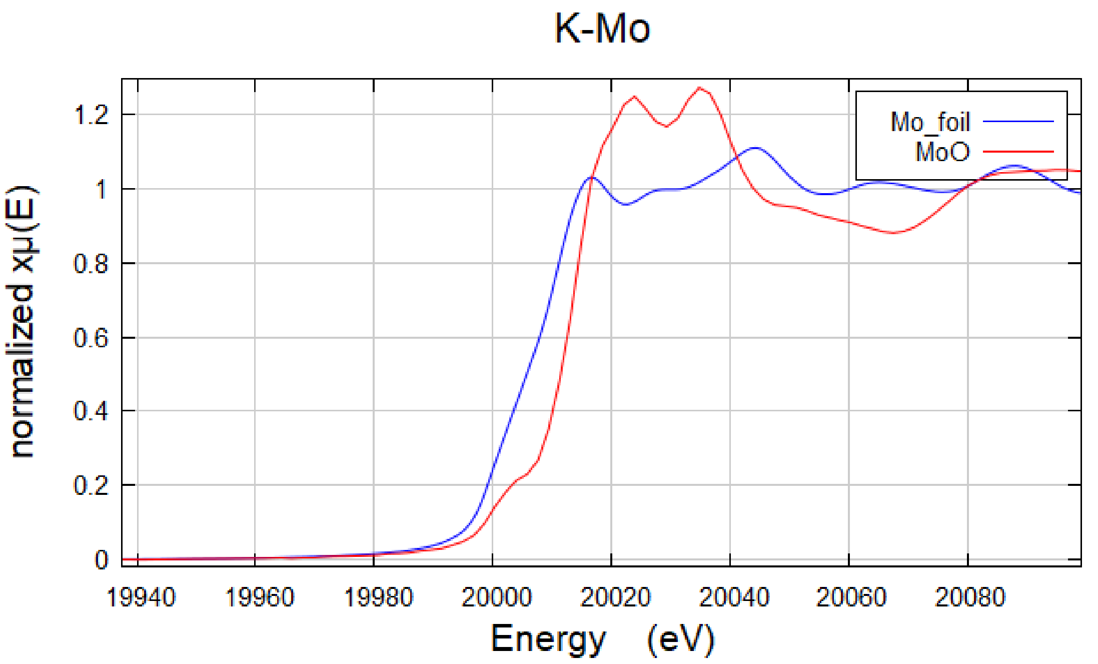

Figure S- 4 **Analyzed XANES Spectra of Mo-K edge**

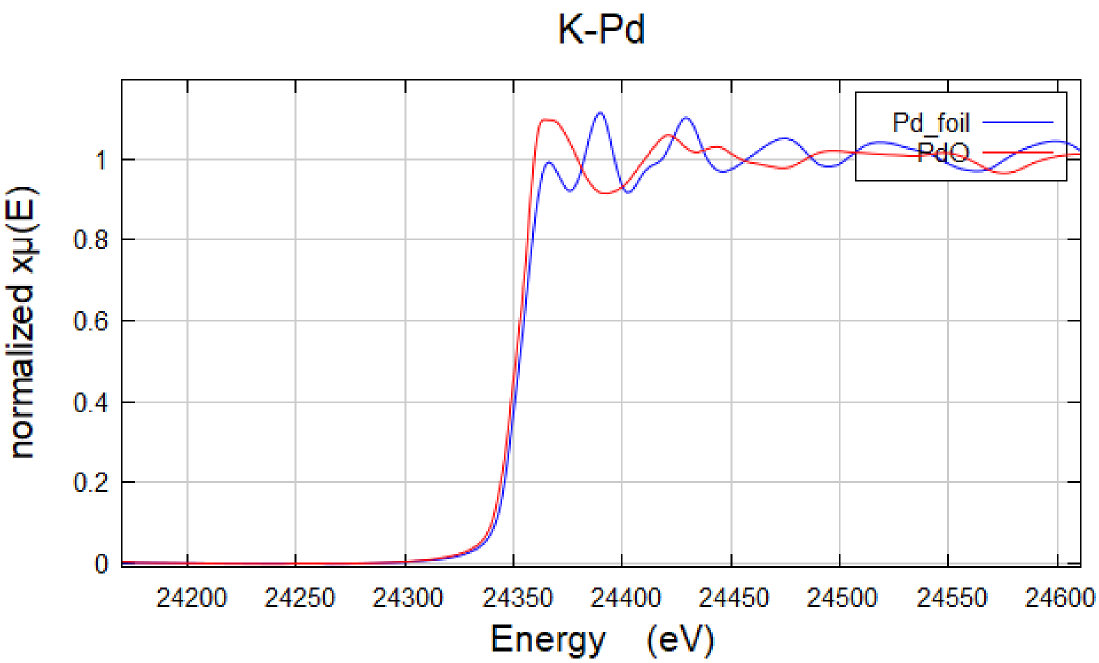

Figure S- 5 **Source XANES Spectra for data mining (Pd-K edge)**

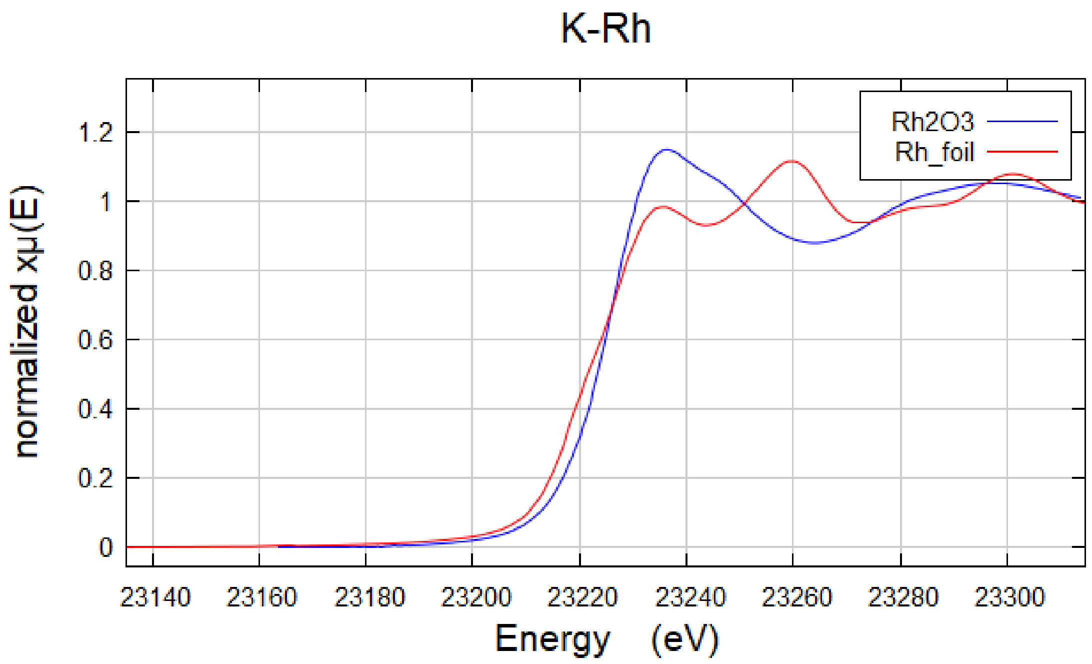

Figure S- 6 **Source XANES Spectra for data mining (Rh-K edge)**

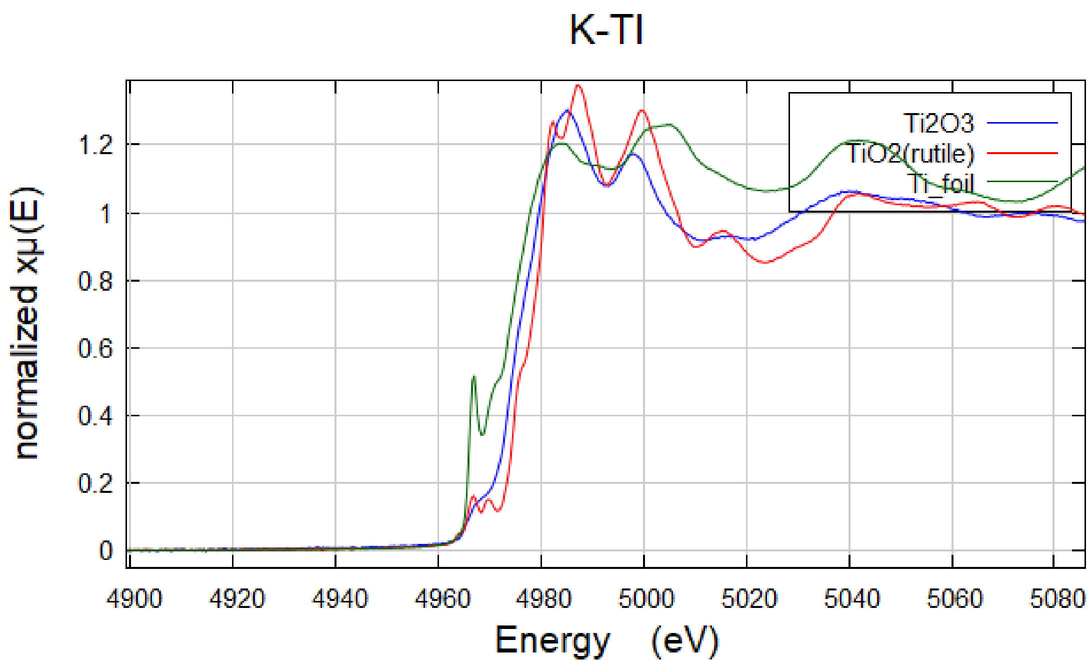

Figure S- 7 **Source XANES Spectra for data mining (Ti-K edge)**

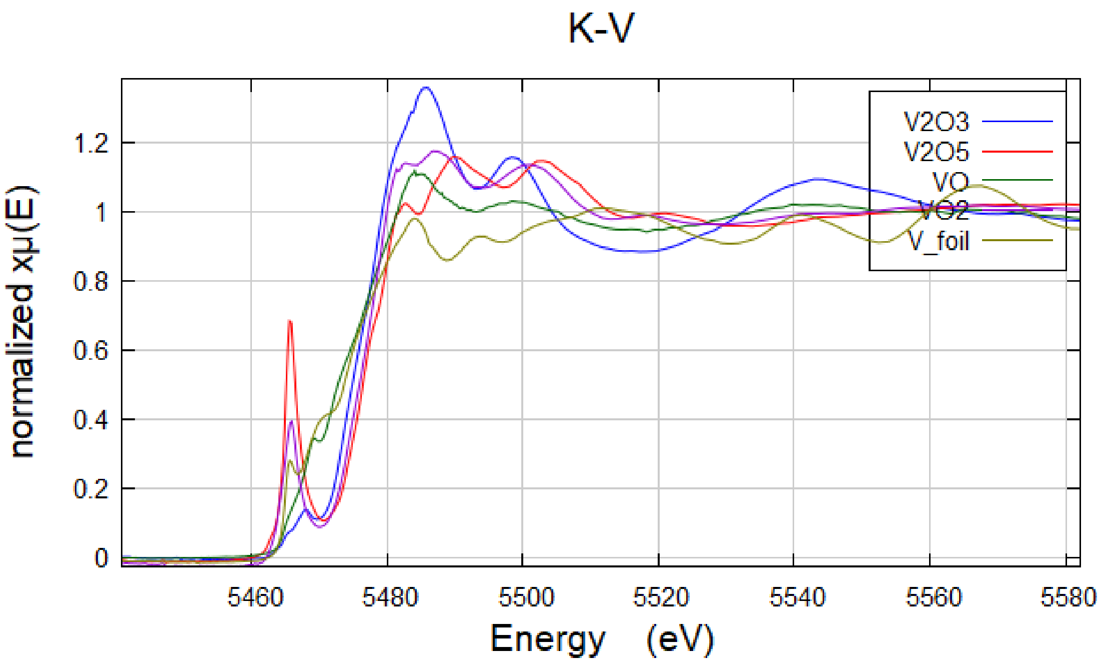

Figure S- 8 **Source XANES Spectra for data mining (V-K edge)**

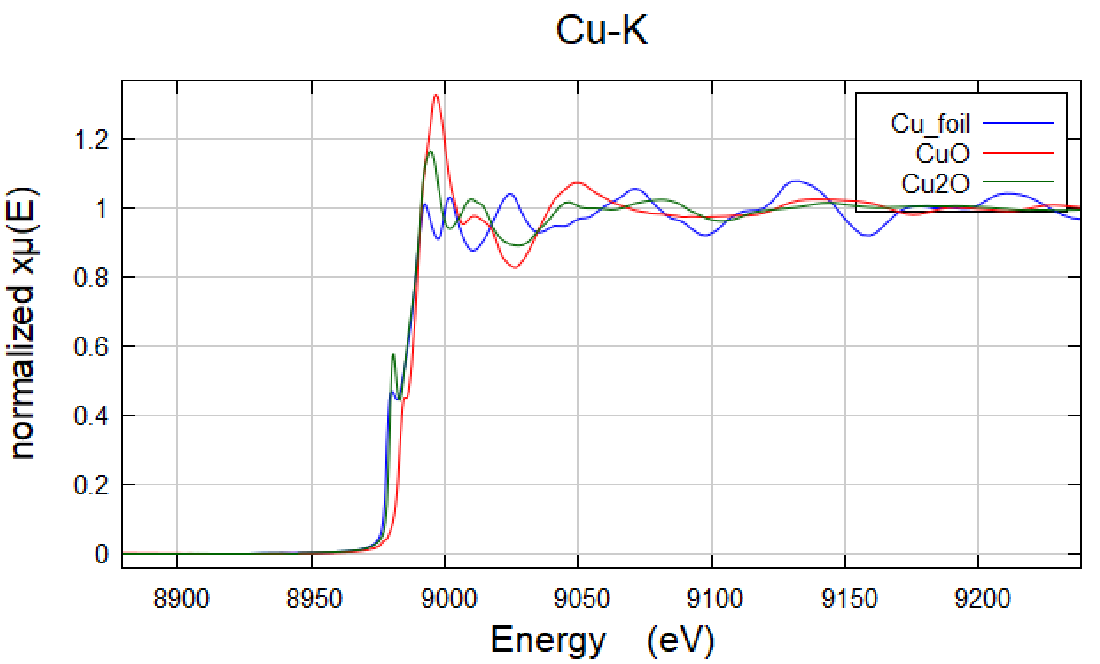

Figure S- 9 **Source XANES Spectra for** oxidation state prediction **(Cu-K edge)**

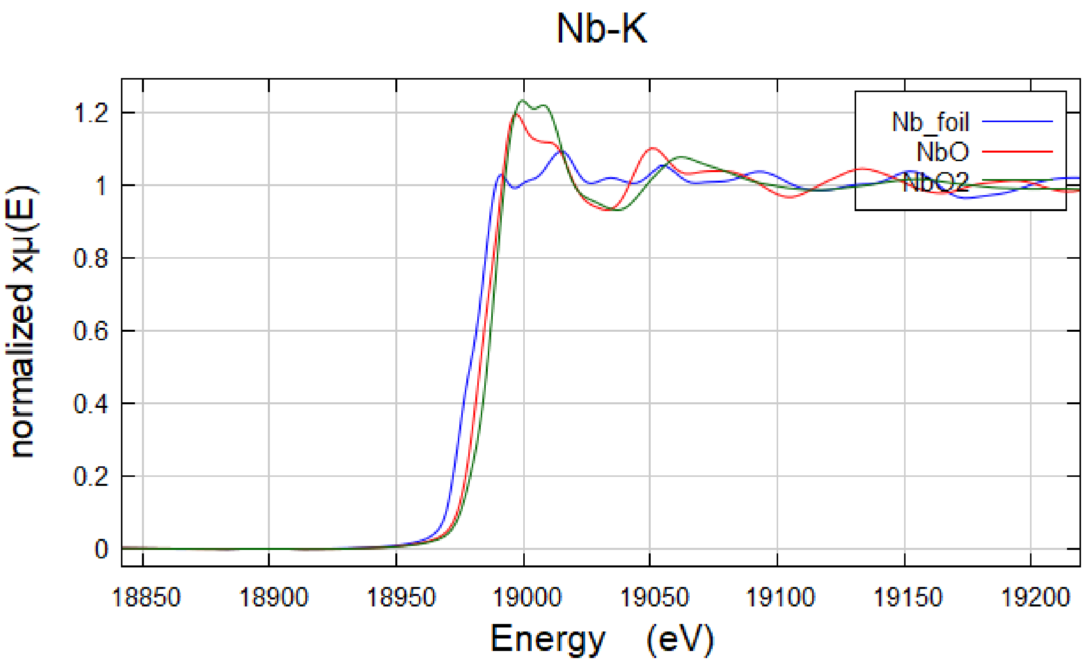

Figure S- 10 **Source XANES Spectra for** oxidation state prediction **(Nb-K edge)**

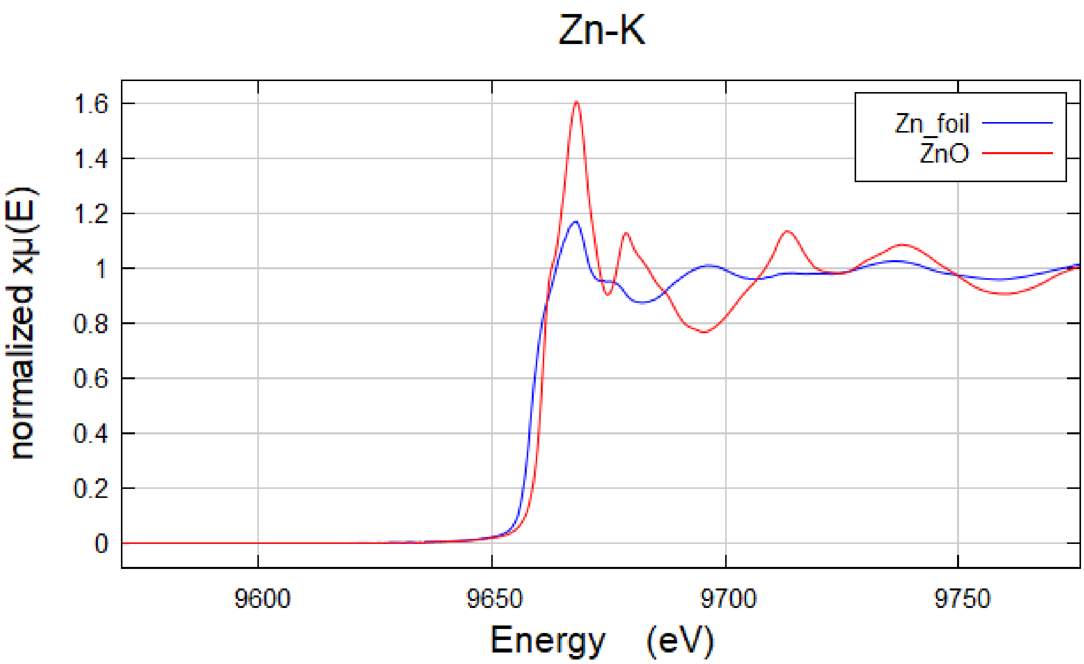

Figure S- 11 **Source XANES Spectra for** oxidation state prediction **(Zn-K edge)**

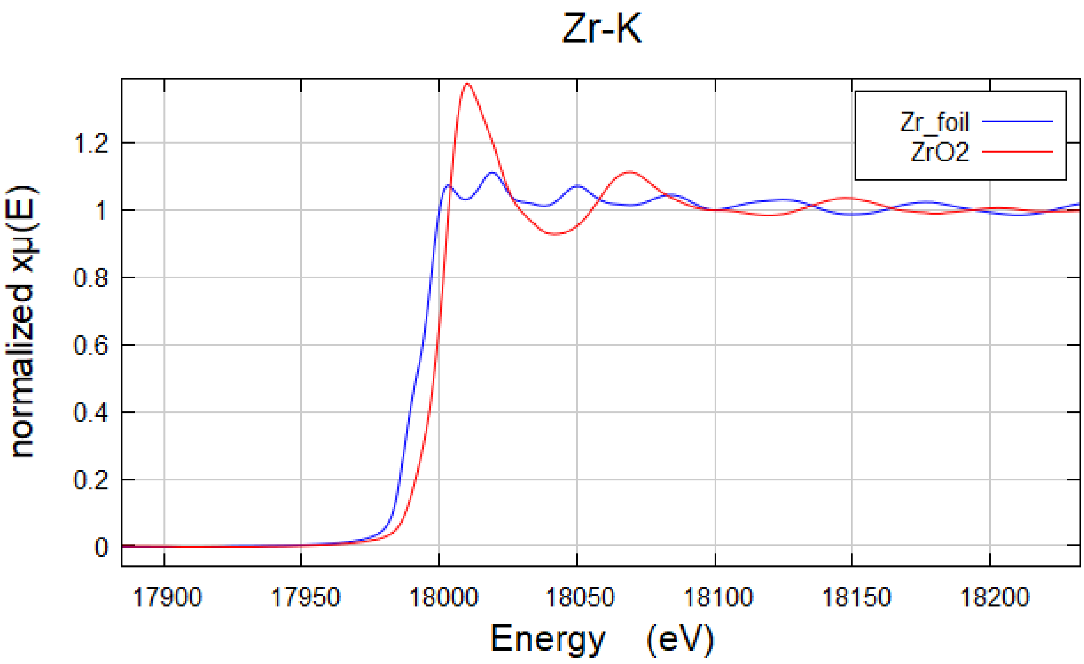

Figure S- 12 **Source XANES Spectra for** oxidation state prediction **(Zr-K edge)**

Table S- 1 The list of learned data for data mining.

Name of Oxide	O_{stat}	O_{clasa} (Target)	Edge	T_{atom}	Trained descriptors									
					T_{num}	$\Delta\mu(E)_{0.1}$	$\Delta\mu(E)_{0.2}$	$\Delta\mu(E)_{0.3}$	$\Delta\mu(E)_{0.4}$	$\Delta\mu(E)_{0.5}$	$\Delta\mu(E)_{0.6}$	$\Delta\mu(E)_{0.7}$	$\Delta\mu(E)_{0.8}$	$\Delta\mu(E)_{0.9}$
Ag foil	0	0	K	Ag	47	67.86	71.60	73.80	75.49	77.34	79.40	81.50	83.35	85.65
Ag_2O	1	0	K	Ag	47	67.83	71.57	73.44	74.82	76.35	78.16	80.34	82.58	85.01
Co_3O_4	2.5	1	K	Co	27	55.55	57.63	58.85	59.93	61.11	62.17	63.01	63.88	65.16
CoO	2	1	K	Co	27	36.12	38.08	39.32	40.39	41.43	42.34	43.24	43.89	44.53
Co foil	0	0	K	Co	27	46.09	47.65	48.96	51.58	54.44	55.91	57.68	59.58	61.51
Fe_2O_3	3	2	K	Fe	26	53.09	55.14	56.00	56.78	57.51	58.27	59.05	59.71	60.33
Fe foil	0	0	K	Fe	26	44.67	46.02	47.71	51.48	53.02	54.32	55.73	57.98	61.10
Fe_3O_4	2.5	1	K	Fe	26	54.32	56.39	57.53	58.50	59.43	60.28	61.07	61.94	62.88
FeO	2	1	K	Fe	26	51.59	53.98	55.01	55.88	56.70	57.67	58.54	59.28	59.97
MoO	2	1	K	Mo	42	52.95	57.59	62.54	64.36	65.71	66.87	67.82	68.76	69.74
Mo foil	0	0	K	Mo	42	57.50	60.26	62.45	64.67	66.89	69.01	70.79	72.34	73.89
Pd foil	0	0	K	Pd	46	66.94	71.15	73.68	75.90	78.06	80.12	82.09	84.10	86.52
PdO	2	1	K	Pd	46	67.26	71.47	74.25	76.35	78.41	80.46	82.27	83.83	85.32
Rh foil	0	0	K	Rh	45	40.88	45.00	47.62	49.69	52.00	54.55	56.78	58.83	61.33
Rh_2O_3	3	2	K	Rh	45	43.00	47.37	50.11	52.27	53.82	55.33	56.71	58.03	59.53
Ti foil	0	0	K	Ti	22	44.98	45.57	45.92	46.33	46.82	53.30	54.35	55.42	56.64
TiO_2	4	2	K	Ti	22	44.02	51.66	52.58	53.24	54.07	55.84	56.84	57.66	58.33
Ti_2O_3	3	2	K	Ti	22	46.87	51.55	53.23	54.16	55.01	55.89	56.96	58.15	59.36
V foil	0	0	K	V	23	2.18	2.74	5.90	8.08	11.32	12.69	14.39	16.46	18.87
VO_2	4	2	K	V	23	1.63	2.42	3.06	12.95	13.88	14.77	15.61	16.41	17.17
VO	2	1	K	V	23	13.76	15.78	17.14	20.05	21.38	23.21	24.99	26.61	28.39
V_2O_5	5	2	K	V	23	3.69	4.48	4.76	5.04	5.32	6.20	18.66	19.73	20.59
V_2O_3	3	2	K	V	23	5.00	10.47	11.48	12.34	13.25	14.20	15.16	16.08	16.87

Table S- 2 The list of data used for oxidation state prediction.

Name of Oxide	Trained descriptors									
	T_{num}	Δμ(E)=0.1	Δμ(E)=0.2	Δμ(E)=0.3	Δμ(E)=0.4	Δμ(E)=0.5	Δμ(E)=0.6	Δμ(E)=0.7	Δμ(E)=0.8	Δμ(E)=0.9
Cu-foil	29	7.49671	8.65836	9.47834	10.23596	15.0762	17.17498	18.79599	20.15169	21.3928
CuO	29	11.61854	13.15497	14.06559	15.45102	17.93745	19.10673	20.09161	20.79723	21.50284
Cu_2O	29	45.94438	49.25226	52.17972	54.42547	56.03967	57.25297	58.32525	59.23256	60.1393
Nb-foil	41	34.87828	37.75439	39.89872	41.93509	44.44644	46.94628	48.83271	50.56057	52.24945
NbO	41	39.27371	42.65305	44.86342	46.6414	48.33328	50.02334	51.83187	53.64515	55.36128
NbO2	41	40.51781	44.50858	47.34046	49.44839	51.13021	52.5735	53.88183	55.1746	56.51443
Zn-foil	30	29.87923	31.27251	31.99473	32.71694	33.34076	33.95263	34.5645	35.63119	36.88523
ZnO	30	31.63073	33.19231	33.96574	34.69648	35.07969	35.4629	35.8461	36.22931	36.7778
Zr-foil	40	40.49092	42.72216	44.11548	45.43669	48.89947	51.14169	52.50997	53.74389	54.96115
ZrO2	40	45.94438	49.25226	52.17972	54.42547	56.03967	57.25297	58.32525	59.23256	60.1393