

APPENDIX A. SUPPLEMENTARY MATERIALS

Yu Lu

Table 1 records the exact results and parameters for background subtractions.

Table 2 records all the results of sulfur speciation in petroleum asphaltene, using different normalization parameters and methods.

Table 1

Peak Energy of all spectra, pre-tail energy range used when performing background subtraction, and the coefficient of determination of linear regression.

Name	Peak Energy/eV	Pre-tail Energy Range/eV (# of points)	R^2 for regression
Petroleum Asphaltene	2473.15	2422-2466(20)	0.857
DBS	2472.4	2414-2453(20)	0.808
DBT	2473	2461-2465(20)	0.617
DBSO	2475.2	2458-2462(20)	0.119
DBSO ₂	2478.55	2466-2470(20)	0.884
FeSO ₄	2481.6	2464-2468(20)	0.644

Table 2

All speciation results and their parameters. The “Method” column records the fitting method (DF for deconvolution fitting and LCF for linear combination fitting) and the degree of the polynomial used in the regression of post-tail during normalization. For example, LCF-1 stands for linear combination fitting with a linear regression model for post-tail fitting in normalization.

Method	Post-edge Energy Range	DBS	DBT	DBSO	DBSO ₂	FeSO ₄	χ^2
LCF-0	2500-2510	1.04%	87.19%	1.89%	4.01%	5.85%	7.07
LCF-0	2500-2515	0.34%	91.80%	1.02%	2.22%	4.62%	6.77
LCF-0	2500-2525	0.16%	94.90%	0.73%	0.62%	3.58%	5.71
LCF-0	2510-2515	0.19%	97.20%	0.45%	0.01%	2.20%	5.08
LCF-0	2510-2525	0.27%	95.50%	1.82%	0.14%	2.27%	3.59
LCF-0	2510-2535	0.27%	95.30%	1.95%	2.23%	2.23%	3.41
LCF-0	2515-2520	0.44%	92.70%	3.55%	0.83%	2.45%	2.63
LCF-0	2515-2525	0.40%	93.40%	3.14%	0.65%	2.39%	2.78
LCF-0	2520-2525	0.37%	94.10%	2.74%	0.47%	2.32%	2.96
LCF-1	2520-2570	0.62%	93.00%	3.72%	1.64%	1.00%	2.99
LCF-1	2520-2560	0.58%	94.50%	2.60%	1.45%	0.89%	3.97
LCF-1	2520-2550	0.78%	92.40%	4.48%	0.74%	1.56%	2.92
LCF-1	2520-2540	0.96%	91.50%	4.52%	0.74%	2.29%	2.40
LCF-1	2520-2530	9.96%	75.60%	9.23%	2.43%	2.74%	2.24
LCF-1	2510-2570	0.44%	94.80%	2.19%	1.38%	1.19%	4.29
LCF-1	2510-2560	0.44%	95.60%	1.32%	1.31%	1.33%	5.49
LCF-1	2510-2550	0.46%	95.30%	1.71%	0.59%	1.93%	5.44
LCF-1	2510-2540	0.41%	95.70%	0.48%	0.60%	2.81%	6.92
LCF-1	2510-2530	12.10%	77.20%	0.84%	0.59%	4.55%	12.56
LCF-2	2510-2570	30.20%	53.80%	2.97%	2.06%	11.00%	15.00
LCF-2	2510-2560	12.60%	69.00%	3.74%	0.40%	14.30%	12.30

LCF-2	2520-2570	11.80%	80.40%	3.70%	0.01%	4.05%	5.56
LCF-2	2520-2560	10.59%	73.60%	11.30%	2.07%	2.46%	2.70
LCF-2	2520-2565	2.37%	86.90%	6.40%	0.01%	4.34%	2.79
DF-0	2505-2515	9.10%	62.07%	14.21%	10.02%	4.60%	0.44
DF-0	2510-2520	5.87%	70.86%	12.44%	7.23%	3.61%	0.34
DF-0	2510-2525	5.58%	71.81%	12.24%	6.90%	3.47%	0.33
DF-0	2510-2530	4.68%	73.50%	11.85%	6.62%	3.34%	0.33
DF-0	2515-2525	7.99%	66.04%	14.79%	6.81%	4.37%	0.53
DF-0	2520-2525	0.26%	76.19%	14.07%	6.02%	3.45%	0.63
DF-1	2510-2530	12.46%	56.53%	16.22%	9.88%	4.91%	0.49
DF-1	2510-2540	11.77%	60.89%	14.96%	8.22%	4.16%	0.44
DF-1	2510-2550	11.52%	62.57%	15.01%	7.60%	3.29%	0.37
DF-1	2510-2560	11.52%	63.09%	14.57%	7.94%	2.87%	0.36
DF-1	2510-2570	10.89%	62.66%	13.54%	12.33%	0.57%	0.50
DF-1	2520-2530	11.81%	59.94%	17.15%	6.00%	5.10%	0.62
DF-1	2520-2540	12.74%	56.09%	22.44%	5.13%	3.60%	0.50
DF-1	2520-2550	9.87%	65.93%	15.07%	6.62%	2.52%	0.32
DF-1	2520-2560	10.91%	65.02%	14.24%	7.64%	2.18%	0.32
DF-1	2520-2570	9.58%	66.41%	14.30%	7.68%	2.03%	0.32
