

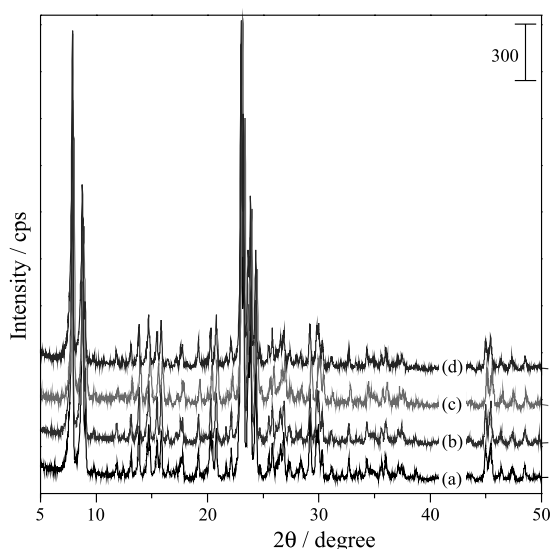
# Supplementary Information

## Characterization of ZSM-5 Modified with Niobium Pentoxide: the Study of Thiophene Adsorption

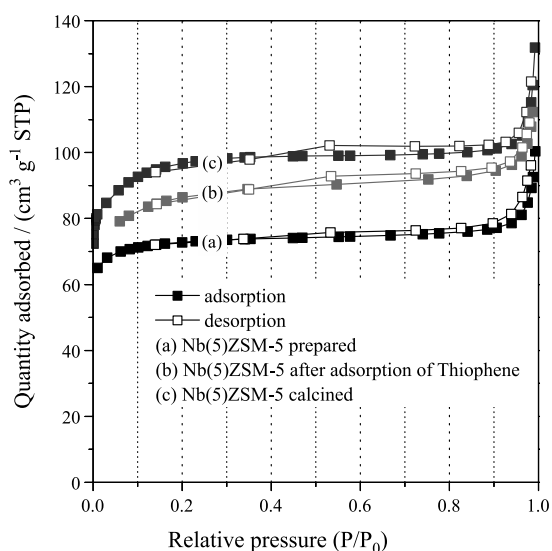
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**Figure S1.** X-ray diffractograms of: (a) pure zeolite ZSM-5, (b) HZSM-5 calcined at 823 K, (c) adsorbent Nb(5)NH<sub>4</sub>ZSM-5 freshly prepared, (d) adsorbent Nb(5)HZSM-5 calcined at 823 K.



**Figure S2.** Nitrogen adsorption isotherms by adsorbent Nb(5)ZSM-5 not calcined (a), after adsorption of thiophene (b) and calcined (c).

**Table S1.** Chemical analysis by XRF of the sulfur concentration in the solution

Reaction time / min	XRF of S (by mass)		
	Solution 2 (C <sub>0</sub> = 605.48 mg L <sup>-1</sup> S)		
	Removal <sup>a</sup> of S / % at 353 K	Removal <sup>a</sup> of S / % at 333 K	Removal <sup>a</sup> of S / % at 301 K
0	ca. 0	ca. 0	ca. 0
10	11.1	19.1	11.5
30	27.8	27.8	8.5
50	47.6	30.3	10.0
60	67.0	32.0	11.5
180	–	28.6	10.4
240	76.4	–	–
300	78.3	–	–
360	74.9	–	–

<sup>a</sup>Calculated from the initial S content of the synthetic fuel.

**Table S2.** Error functions used for the analysis of the kinetic modeling

Error functions	Abbreviation	Formula	Reference
The sum of the square of the errors	SSE	$\sum_{i=1} (q_{t,cal} - q_{t,exp})_i^2$	–
The sum of the absolute errors	SAE	$\sum_{i=1}  q_{t,cal} - q_{t,exp} _i$	–
Chi-square	$\chi^2$	$\sum_{i=1} \left[ \frac{(q_{t,exp} - q_{t,cal})^2}{q_{t,cal}} \right]_i$	1
The average relative error	ARE	$\frac{100}{n} \sum_{i=1} \left  \frac{(q_{t,exp} - q_{t,cal})}{q_{t,exp}} \right _i$	2
The normalized standard deviation	$\Delta q / \%$	$100 \sqrt{\frac{\sum_{i=1}^n \left[ \frac{(q_{t,exp} - q_{t,cal})}{q_{t,exp}} \right]^2}{(n-1)}}$	3
The hybrid fractional error function	HYBRID	$\frac{100}{n-p} \sum_{i=1}^n \left[ \frac{(q_{t,exp} - q_{t,cal})}{q_{t,exp}} \right]_i$	4, 5
Marquardt's percent standard deviation	MPSD	$100 \sqrt{\frac{1}{n-p} \sum_{i=1}^n \left[ \frac{(q_{t,exp} - q_{t,cal})}{q_{t,exp}} \right]^2}$	4, 5

**Table S3.** Results of the seven different error analyses of the kinetic models for adsorption of sulfur at different temperatures

	PFOE	PSOE	Elovich	Intra-particle dif.	Bangham
353 K					
SQE	96.3629	150.6094	213.4506	23.9394	272.8390
SEA	20.6615	23.3825	29.6631	12.6878	31.2215
$\chi^2$	4.0518	5.6146	9.0172	0.1680	10.2643
MER	16.2521	14.1018	25.4906	8.3604	17.2483
$\Delta q / \%$	25.3906	20.0880	45.4008	13.1958	24.5579
HYBRID	-16.0948	-3.9873	-24.9369	-5.6615	-3.6640
MPSD	27.8140	22.0053	49.7340	14.4552	26.9019
333 K					
SQE	12.9095	37.3408	16.5559	2.9408	19.2505
SEA	7.1138	9.2700	8.7373	3.6868	9.4418
$\chi^2$	0.9359	2.1591	0.9862	0.7198	1.1174
MER	8.9816	13.7238	10.9280	4.2722	11.5742
$\Delta q / \%$	11.6531	25.3625	13.0677	6.0677	13.4970
HYBRID	14.9693	-13.2103	-2.4275	2.0401	-1.3587
MPSD	13.4558	29.2861	15.0893	7.0064	15.5850
301 K					
SQE	24.9380	2.6953		42.1199	1.7947
SEA	7.3238	3.2672		9.2097	2.7200
$\chi^2$	10.6056	0.4508		6.6423	0.2862
MER	21.8640	10.1729		9.1559	8.6537
$\Delta q / \%$	35.8903	12.4189		10.9569	10.6337
HYBRID	27.7269	1.6975		-1.7924	-0.8373
MPSD	41.4426	14.3401		12.6520	12.2787

## References

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