

W/Mo-Oxide Nanomaterials:

Structure-Property Relationships and Ammonia Sensing Studies

Ying Zhou¹, Kaibo Zheng^{2, 3}, Jan-Dierk Grunwaldt⁴, Thomas Fox¹, Leilei Gu², Xiaoliang Mo²,
Guorong Chen², Greta. R. Patzke^{1*}

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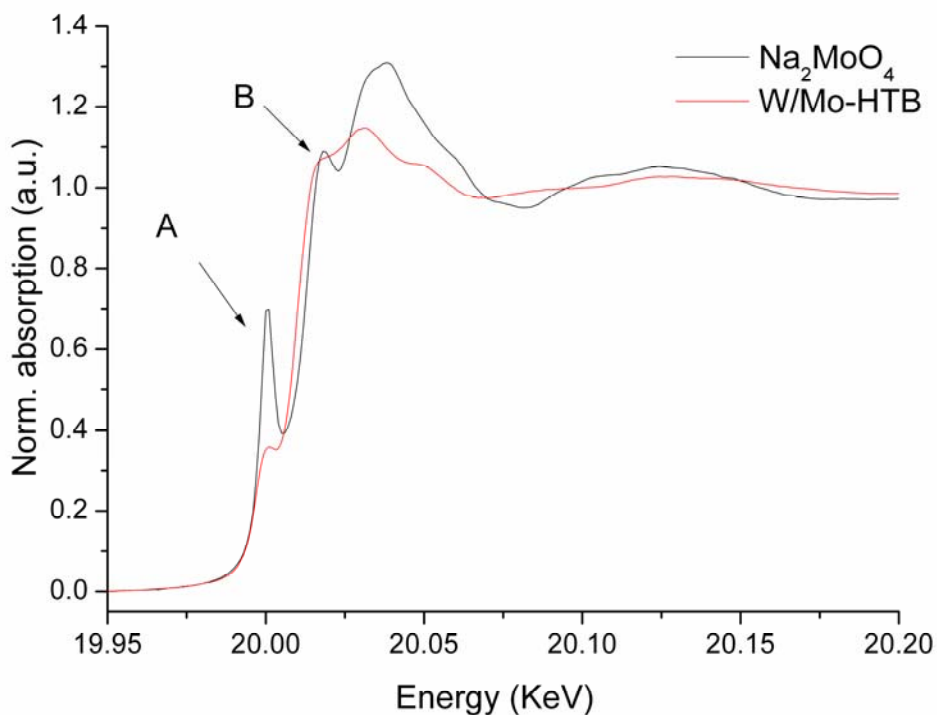


Figure S1. Comparison of representative Mo K-edge XANES spectra of W/Mo-HTB-oxide and Na_2MoO_4 as a reference compound containing tetrahedrally coordinated Mo(VI).

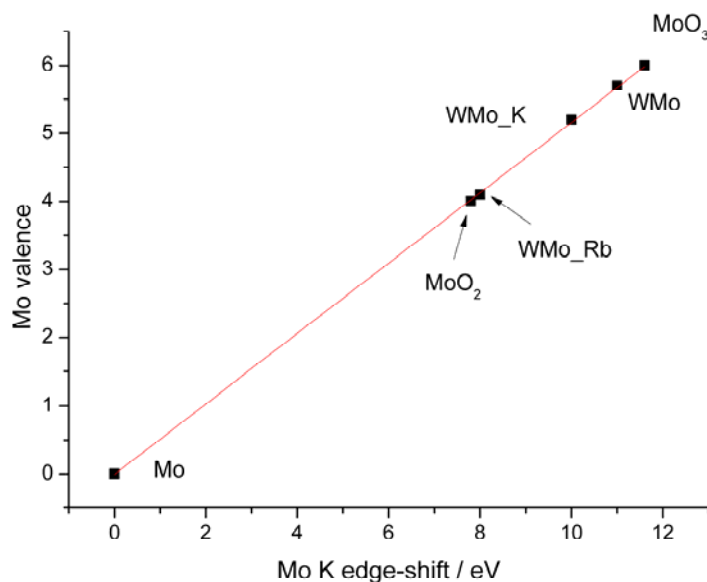


Figure S2. Linear relationship of the average Mo valence and the corresponding Mo K-edge positions.

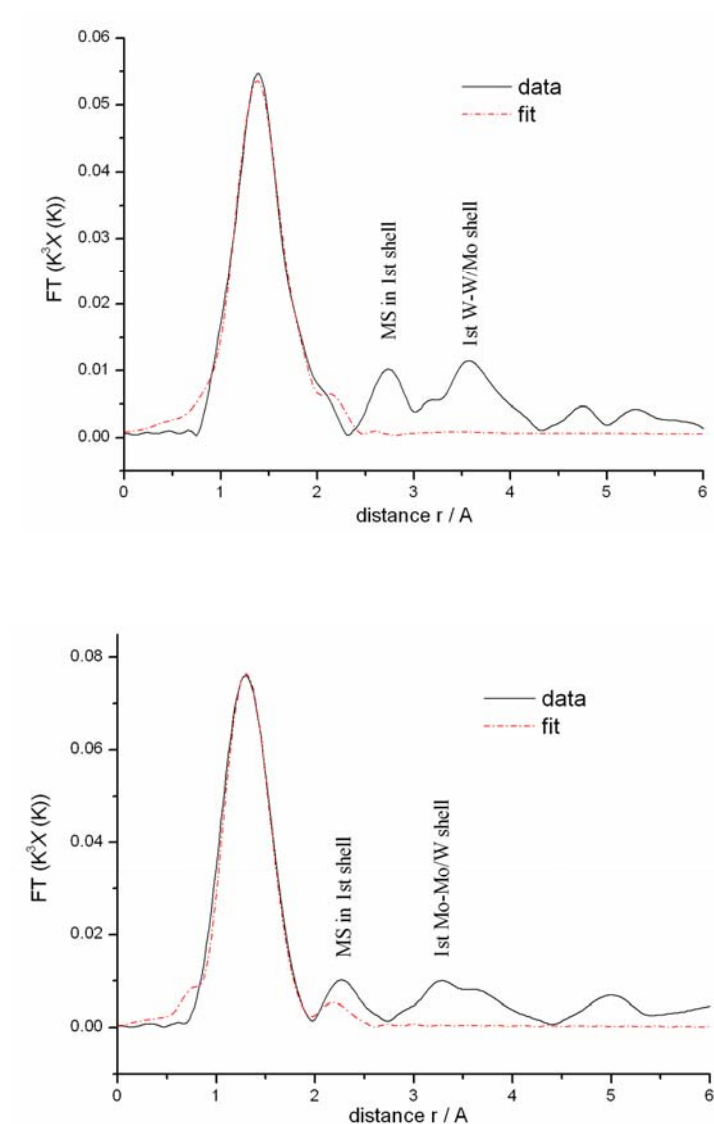


Figure S3. Representative first-shell fit of a W/Mo-HTB sample, considering the nearest oxygen neighbours (a) recorded at the W L₃-edge and (b) recorded at the Mo K-edge.

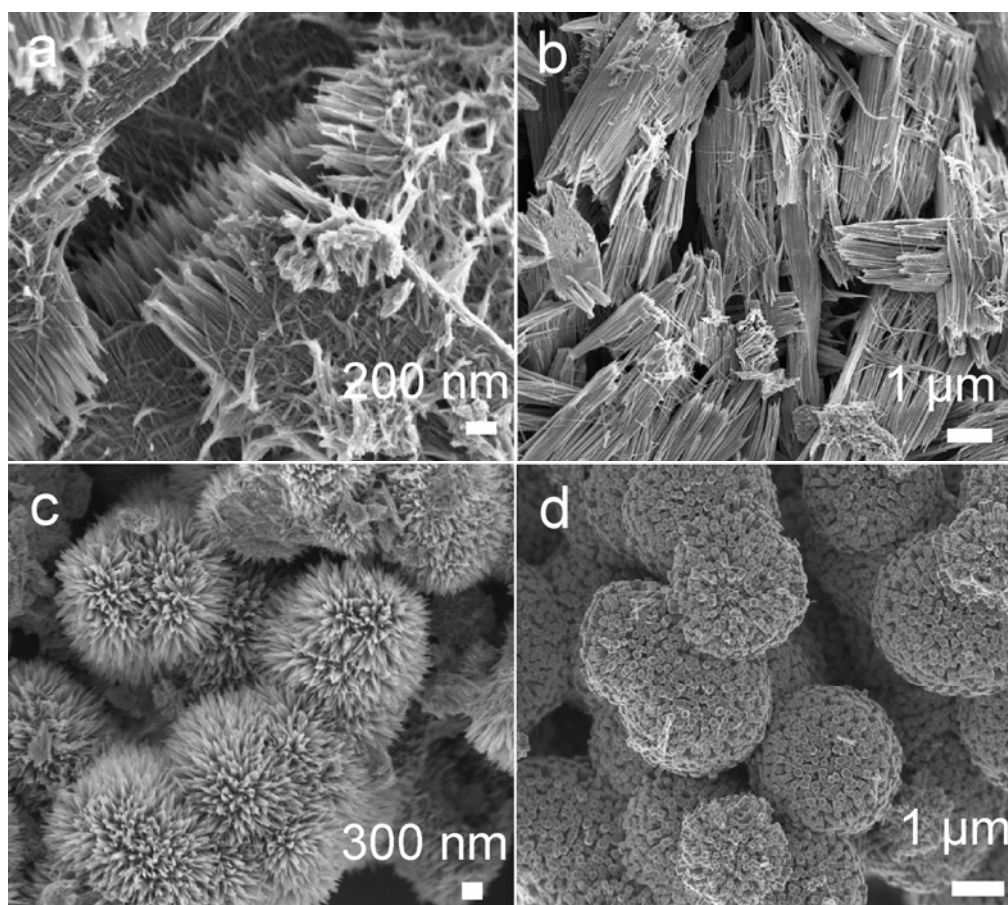


Figure S4. Representative SEM images of W/Mo-HTB samples before heat treatment: (a) Li_W/Mo-HTB; (b) Na_W/Mo-HTB; (c) K_W/Mo-HTB; (d) Rb_W/Mo-HTB.

Table S1 Structural parameters derived from fitting of EXAFS spectra at the W L₃-edge of M-WMo-HTBs (W-O bonds; M = Li - Rb).*

Samples	N	$R / \text{\AA}$	$\delta^2 / \text{\AA}^2$	$\Delta E / eV$	Residual
WMo	2.3	1.73	0.004	12.2	7.0
	1.9	1.83	0.004	12.4	
	1.8	2.06	0.004	12.5	
WMo_Li	2.2	1.74	0.004	12.1	8.8
	2.6	1.87	0.010	12.2	
	1.2	2.10	0.002	12.2	
WMo_Na	2.7	1.75	0.006	12.2	9.9
	1.4	1.81	0.004	12.2	
	1.9	2.06	0.006	12.3	
WMo_K	2.4	1.74	0.003	12.4	7.0
	1.8	1.89	0.006	12.5	
	1.8	2.07	0.003	12.6	
WMo_Rb	2.0	1.73	0.002	12.9	6.6
	2.4	1.87	0.006	13.1	
	1.6	2.09	0.003	13.2	

* N = coordination number with the overall number 6, R = distance of the first oxygen coordination shell, δ^2 = Debye-Waller factor, ΔE = energy shift and Residual = factor for the goodness of fit

Table S2. Structural parameters obtained from fitting of EXAFS spectra recorded at the Mo K-edge of M-WMo-HTBs (Mo-O bonds; M = Li - Rb).

Samples	N	$R / \text{\AA}$	$\delta^2 / \text{\AA}^2$	$\Delta E / eV$	Residual
WMo	2.5	1.69	0.002	-6.6	5.8
	1.3	1.80	0.005	8.9	
	2.2	2.11	0.005	9.6	
WMo_Li	2.0	1.72	0.001	9.1	5.8
	2.2	1.78	0.003	-12	
	1.8	2.11	0.003	12	
WMo_Na	2.2	1.73	0.001	11.9	4.6
	2.3	1.80	0.004	-12	
	1.5	2.11	0.003	12	
WMo_K	2.1	1.73	0.001	12	5.0
	2.1	1.79	0.003	-12	
	1.8	2.09	0.005	12	
WMo_Rb	2.0	1.71	0.001	9.3	7.3
	2.4	1.78	0.004	-12	
	1.6	2.10	0.005	12	

The mean W/Mo-distances, R_m , were obtained from the following equation:

$$R_m = ((N_1R_1 + N_2R_2 + N_3R_3) / 6).$$

The W-O R_m range varied from 1.86 to 1.88 Å over the entire W/Mo-HTB series, whereas the corresponding Mo-O values covered a slightly shorter distance range between 1.84 and 1.87 Å.

Table S3. Modeling of R–C values (R_b = bulk resistance, R_{gb} and C_{gb} = grain resistance and capacitance, respectively).

T=245 °C	R_b (Ω)	R_{gb} (Ω)	C_{gb} (F)
W/Mo-HTBs	1.567E4	2.032E6	1.891E-11
Li_W/Mo-HTBs	7.319E3	2.571E5	2.831E-11
Na_W/Mo-HTBs	1.533E4	3.372E6	1.537E-11
K_W/Mo-HTBs	1.473E4	2.675E7	1.291E-11
Rb_W/Mo-HTBs	114.8	1.124E7	1.47E-11