Supporting Information for

Wavelet Transform EXAFS Analysis of Mono- and Dimolybdate Model Compounds and a Mo/HZSM-5 Dehydroaromatization Catalyst

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Table S1. WT maxima observed for model molybdates and Mo/HZSM-5

Compound	Feature	k Å^{-1}	R + α Å
$MgMoO_4$	A [a]	5.85	1.18
	B	4.85	2.80
	C	6.80	2.83
	D	8.10	3.05
	E	10.13	3.18
$MgMo_2O_7$	F [a]	5.80	1.14
	G	5.12	2.6 – 2.9
	H	7.00	3.08
	I	7.9 – 8.7	3.0
	J	10.13	3.20
	K	12.85	3.15
Mo/HZM-5	L [a]	6.24	1.08
	M	4.95	2.90
	N	8.68	2.58
	O	11.10	2.82
	P	13.15	2.70

[a] Evaluated using ($\kappa = 3$, $\sigma = 1$), rather than ($\kappa = 5$, $\sigma = 1$).

Table S2. Calculated *R*-space and *q*-space maxima for individual EXAFS paths

Path	FEFF Parameters [a]		Maxima	
	R (Å)	σ^2 (Å^2)	*k* (Å^{-1})[b]	*R* (Å)[c]
Mo-O	1.75	0.0010	5.70	1.41
Mo-O	1.75	0.0015	5.68	1.40
Mo-O	1.75	0.0020	5.51	1.38
Mo-O	1.75	0.0025	5.42	1.36
Mo-O	3.00	0.0010	6.20	2.70
Mo-O	3.00	0.0015	6.17	2.67
Mo-O	3.00	0.0020	6.15	2.64
Mo-O	3.00	0.0025	6.10	2.61
Mo-O-O	3.20	0.0010	3.98	2.70
Mo-O-O	3.20	0.0025	3.92	2.63
Mo-O-O	3.60	0.0010	4.05	3.00
Mo-O-O	3.60	0.0025	3.98	2.98
Mo-O-O	4.70	0.0010	4.07	4.42
Mo-O-O	4.70	0.0025	4.00	4.42
Mo-O-O	4.70	0.0080	3.90	4.43
Mo-Mg	3.30	0.0010	9.20	3.02
Mo-Mg	3.30	0.0025	7.22	2.97
Mo-Mg	3.70	0.0010	8.65	3.41
Mo-Mg	3.70	0.0025	7.80	3.38
Mo-Mg-O	3.50	0.0010	6.70	3.15
Mo-Mg-O	3.50	0.0025	6.15	3.06
Mo-Mg-O	3.80	0.0010	7.20	3.45
Mo-Mg-O	3.80	0.0025	6.60	3.37
Mo-Mo-O	3.60	0.0010	12.65	3.28
Mo-Mo-O	3.60	0.0025	11.10	3.26
Mo-Mo-O	3.75	0.0010	12.85	3.43
Mo-Mo-O	3.75	0.0025	11.15	3.41

Mo-Mo	3.40	0.0010	13.28	3.14
Mo-Mo	3.40	0.0025	11.60	3.13
Mo-Mo	3.50	0.0015	12.70	3.23
Mo-Mo	3.50	0.0020	12.10	3.23
Mo-Mo	3.50	0.0025	11.80	3.23
Mo-Mo	3.50	0.0040	10.40	3.22
Mo-Mo	3.50	0.0060	9.55	3.22
Mo-Mo	3.50	0.0080	9.10	3.22
Mo-Mo	3.50	0.0100	8.50	3.22
Mo-Mo	3.60	0.0010	13.05	3.34
Mo-Mo	3.60	0.0025	12.90	3.33
Mo-Mo	3.60	0.0040	10.30	3.31
Mo-Mo	3.70	0.0010	13.00	3.44
Mo-Mo	3.70	0.0025	11.90	3.43
Mo-Mo	3.70	0.0040	10.49	3.42
Mo-Mo	4.00	0.0010	13.65	3.74
Mo-Mo	4.00	0.0025	12.00	3.73
Mo-Mo	4.00	0.0040	10.50	3.71
Mo-Mo	4.00	0.0080	9.10	3.71
Mo-Mo	4.00	0.0010	8.60	3.71
Mo-Mo	4.70	0.0010	13.5	4.44
Mo-Mo	4.70	0.0040	10.6	4.42
Mo-Mo	4.70	0.0080	9.30	4.39
Mo-Mo	4.70	0.010	8.75	4.39

[a] $\Delta E_0 = 0$ eV. [b] Maximum of q-space magnitude plot. [c] Without phase correction.

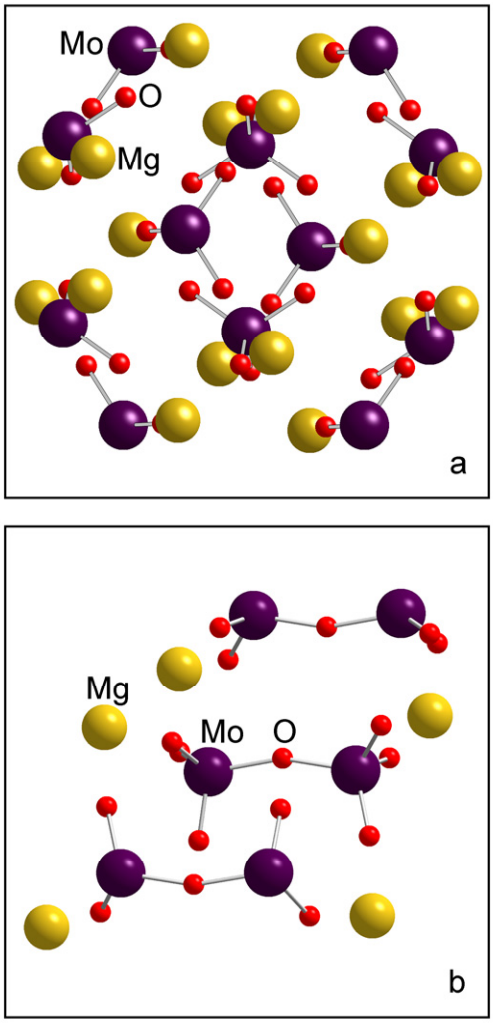

Fig. S1. Crystal structures of (a) $MgMoO_4$, showing isolated MoO_4^{2-} tetrahedra;[1] and (b) $MgMo_2O_7$, showing oxygen-bridged MoO_3 groups.[2]

References

1. V. V. Bakakin, R. F. Klevtsova and L. A. Gaponenko, *Kristallogr.*, 1982, **27**, 38-42.
2. K. Stadnicka, J. Haber and R. Kozlowski, *Acta Cryst.*, 1977, **B33**, 3859-3862.

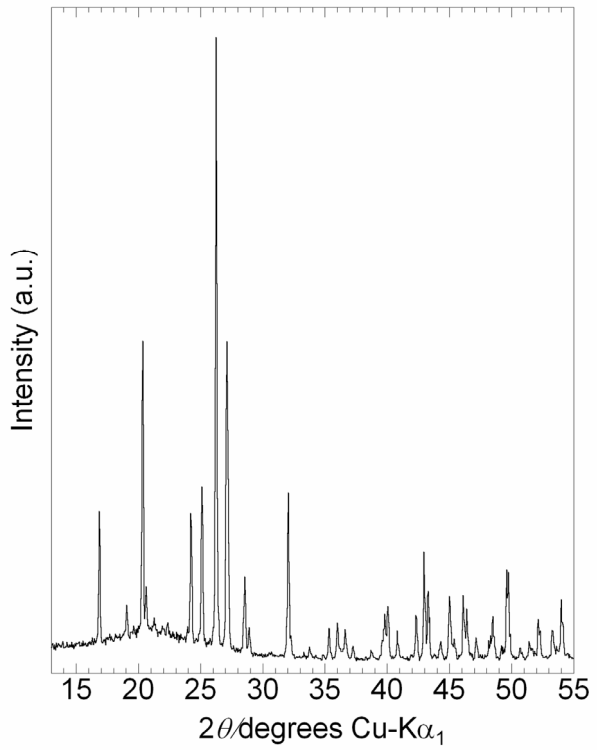

Fig. S2. Powder XRD pattern of $MgMo_2O_7$.

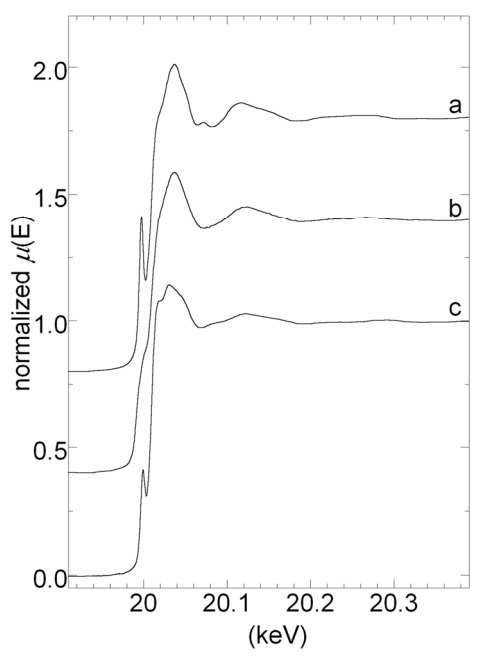

Fig. S3. Raw X-ray absorption spectra, collected in transmission mode at SSRL, for (a) $MgMoO_4$ (BL 4-1), (b) $MgMo_2O_7$ (BL 2-3), and (c) Mo/HZSM-5 (BL 4-1).

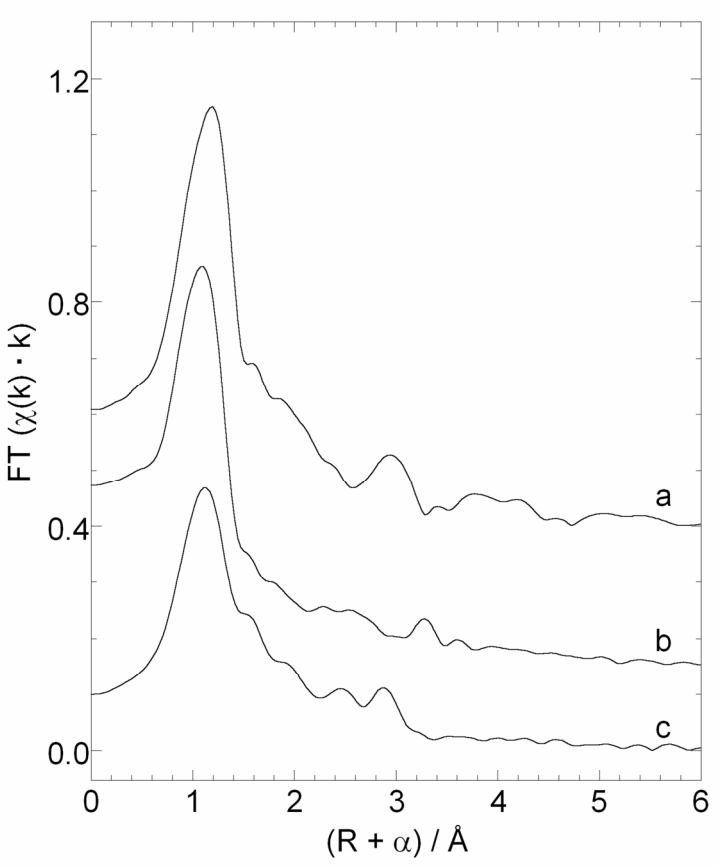

Fig. S4. Comparison of the k^1-weighted EXAFS of (a) $MgMoO_4$, (b) $MgMo_2O_7$, and (c) Mo/HZSM-5.

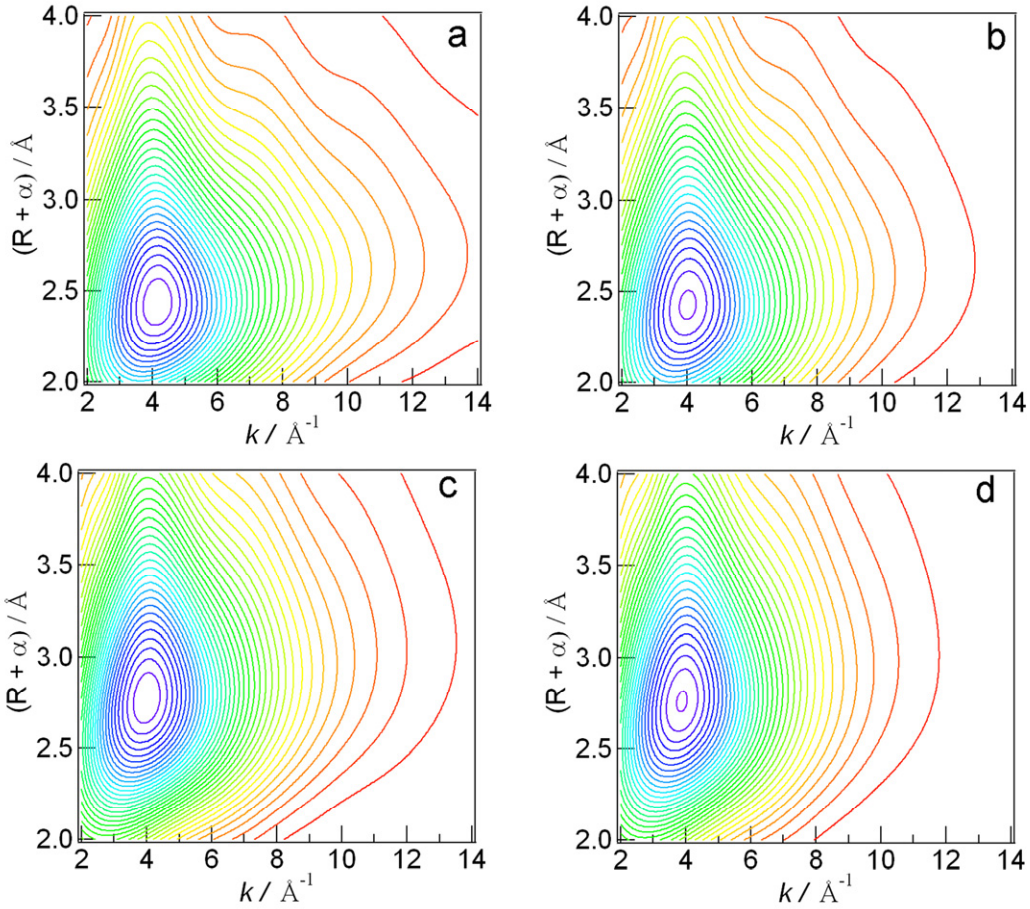

Fig. S5. Calculated WT plots for Mo-O-O paths. See Table S2 for structural parameters.

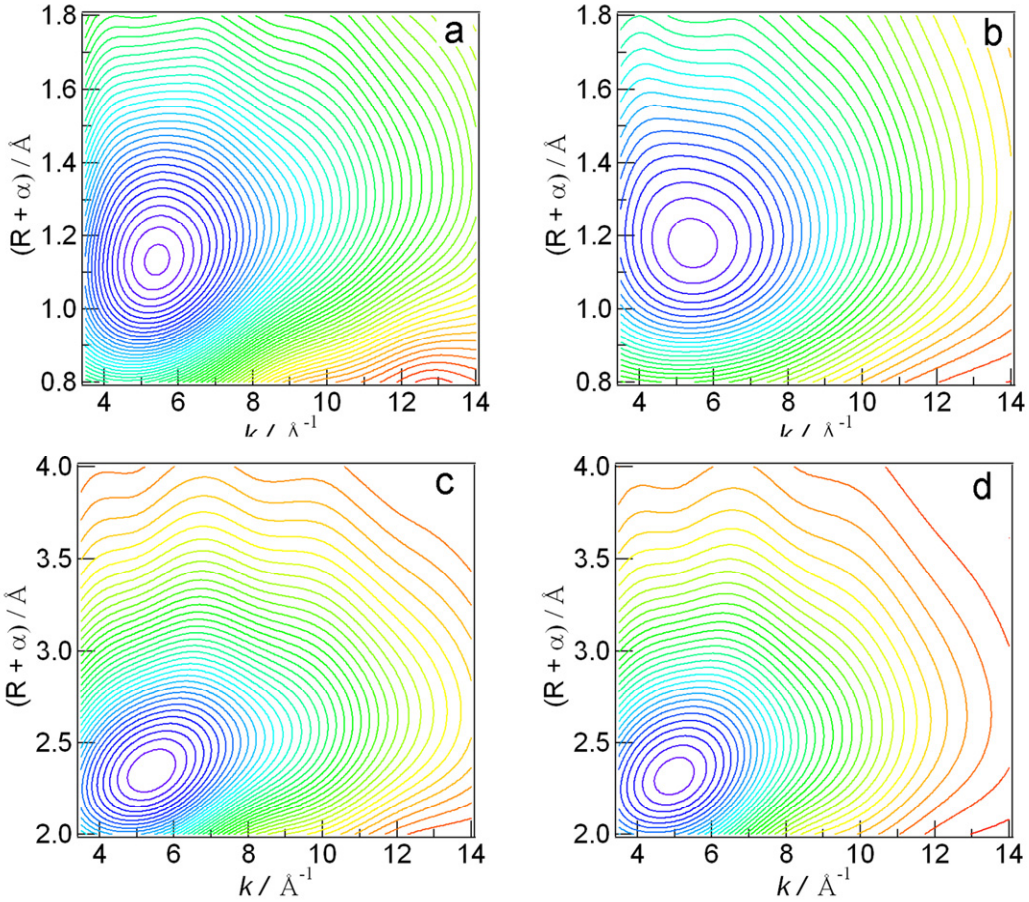

Fig. S6. Calculated WT plots for Mo-O paths. See Table S2 for structural parameters.

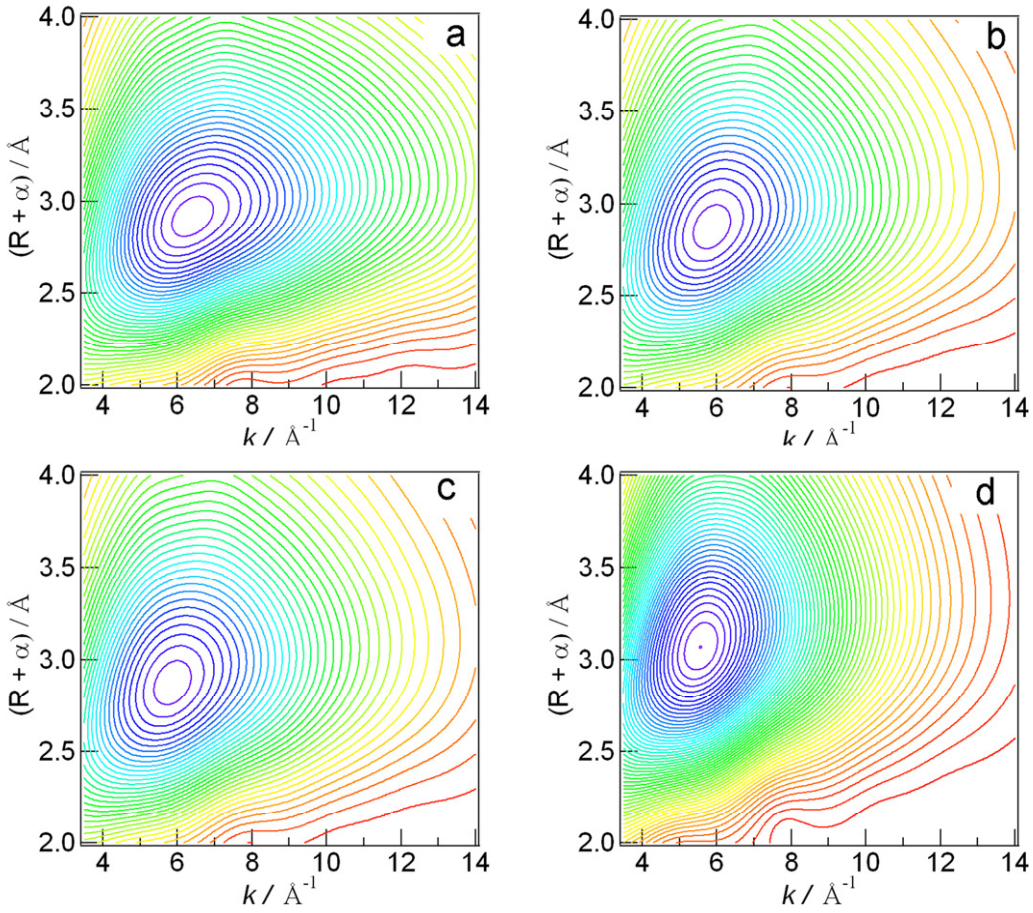

Fig. S7. Calculated WT plots for Mo-Mg-O paths. See Table S2 for structural parameters.

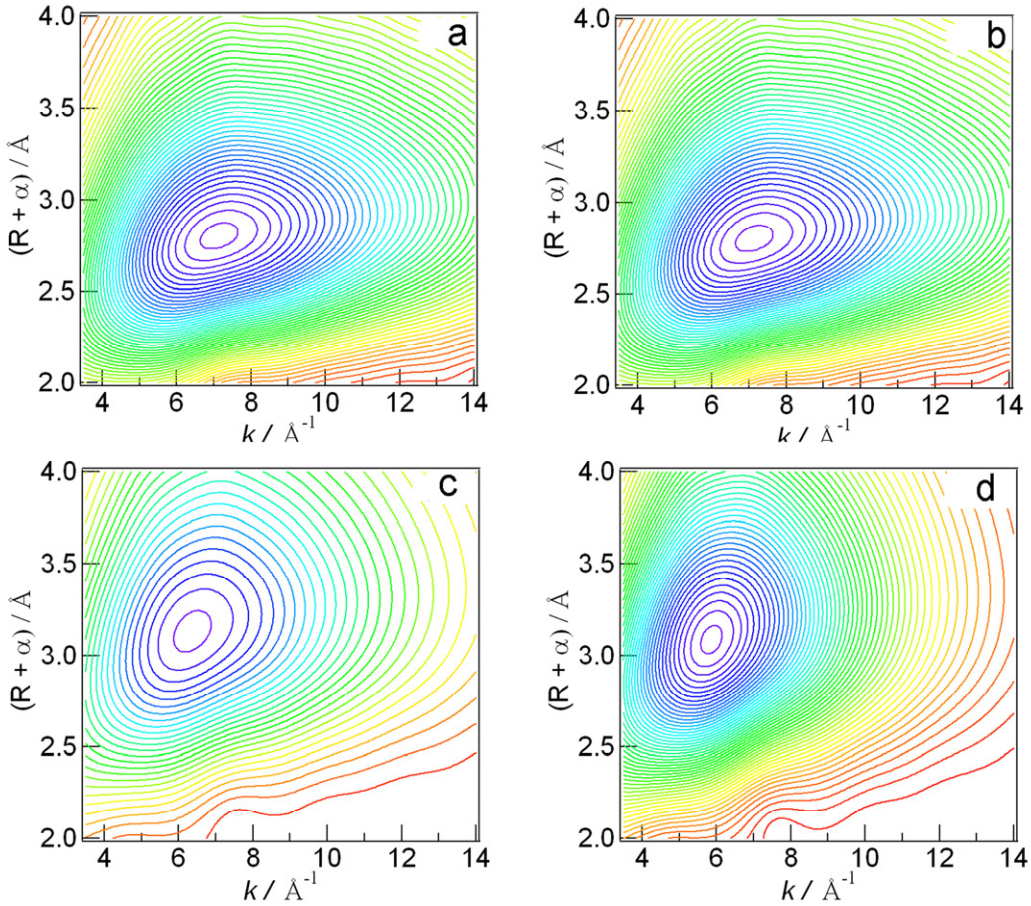

Fig. S8. Calculated WT plots for Mo-Mg paths. See Table S2 for structural parameters.

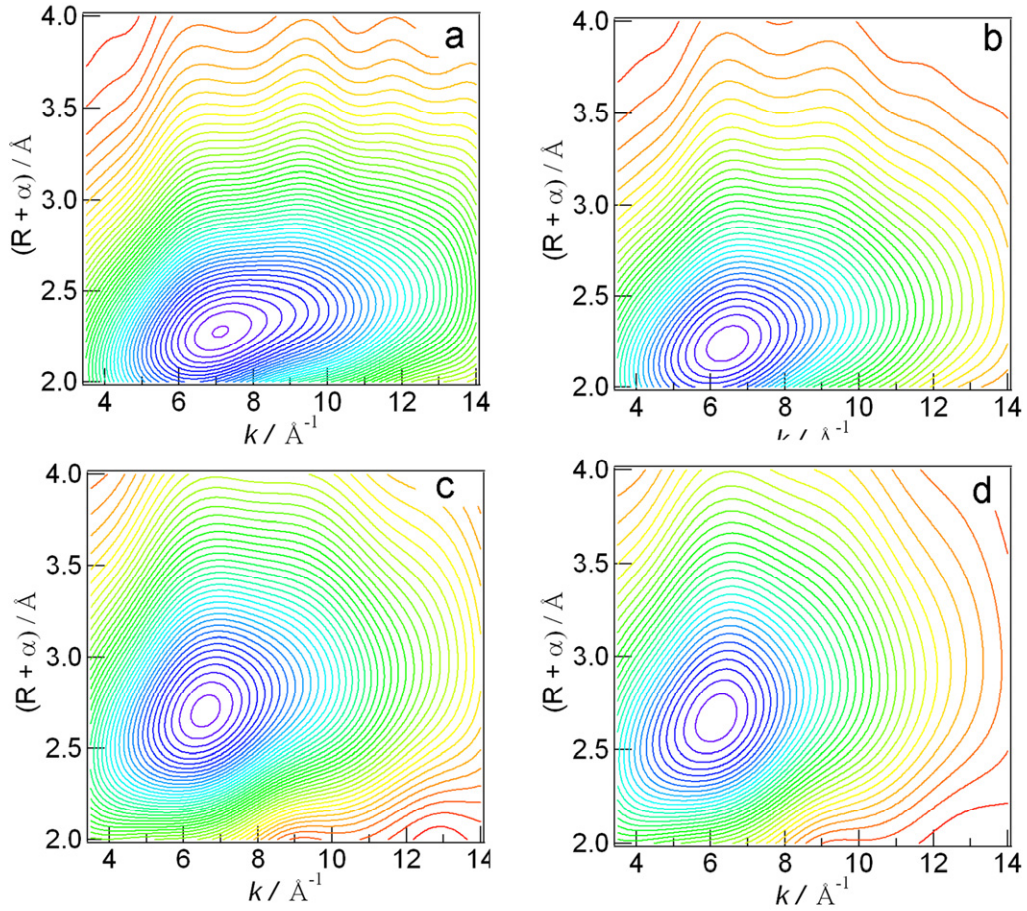

Fig. S9. Calculated WT plots for Mo-Si paths. See Table S2 for structural parameters.

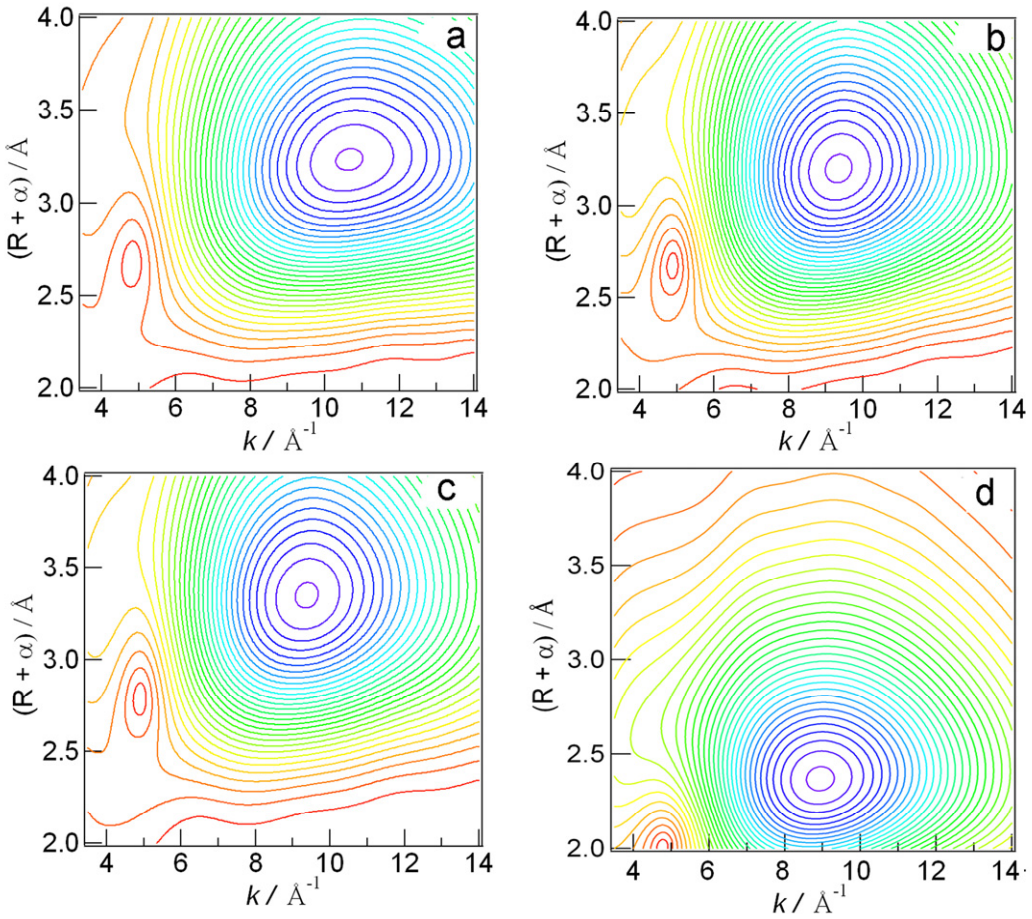

Fig. S10. Calculated WT plots for Mo-Mo-O paths. See Table S2 for structural parameters.

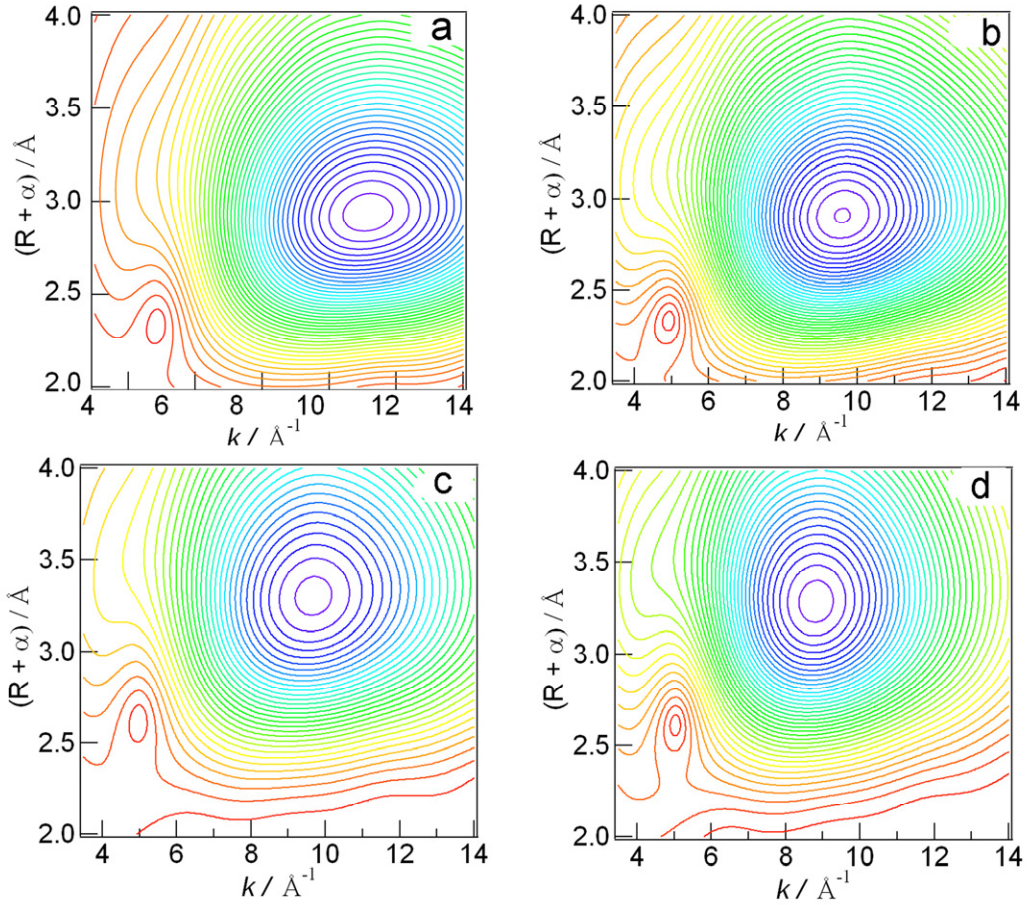

Fig. S11. Calculated WT plots for Mo-Mo paths. See Table S2 for structural parameters.

Table S3. Positions of calculated WT maxima for individual EXAFS paths

Path	FEFF Parameters [a]		Wavelet Transform		Plot [c]
	R (Å)	σ^2 (Å^2)	k (Å^{-1})	R (Å)[b]	
Mo-O-O	3.1	0.003	4.10	2.45	5a
Mo-O-O	3.1	0.006	4.00	2.43	5b
Mo-O-O	3.5	0.006	4.00	2.78	5c
Mo-O-O	3.5	0.009	3.85	2.76	5d
Mo-O	1.7	0.003	5.45	1.14	6a
Mo-O	1.7	0.006	5.40	1.17	6b
Mo-O	3.0	0.006	5.40	2.35	6c
Mo-O	3.0	0.009	5.00	2.30	6d
Mo-Mg-O	3.5	0.003	6.40	2.90	7a
Mo-Mg-O	3.5	0.006	5.90	2.85	7b
Mo-Mg-O	3.75	0.006	5.90	2.88	7c
Mo-Mg-O	3.75	0.009	5.60	3.07	7d
Mo-Mg	3.3	0.003	7.15	2.80	8a
Mo-Mg	3.3	0.006	7.10	2.80	8b
Mo-Mg	3.7	0.006	6.40	3.15	8c
Mo-Mg	3.7	0.009	5.90	3.08	8d
Mo-Si	2.8	0.003	7.15	2.27	9a
Mo-Si	2.8	0.006	6.50	2.23	9b
Mo-Si	3.3	0.006	6.70	2.70	9c
Mo-Si	3.3	0.009	6.15	2.65	9d
Mo-Mo-O	3.65	0.003	10.60	3.24	10a
Mo-Mo-O	3.65	0.006	9.30	3.20	10b
Mo-Mo-O	3.8	0.006	9.40	3.35	10c
Mo-Mo-O	2.8	0.007	8.95	2.35	10d
Mo-Mo	3.3	0.003	11.15	2.93	11a
Mo-Mo	3.3	0.006	9.60	2.91	11b
Mo-Mo	3.7	0.006	9.70	3.30	11c
Mo-Mo	3.7	0.009	8.80	3.30	11d

[a] $\Delta E_0 = 0$ eV. [b] Without phase correction. [c] See Figs. S5 - S11.

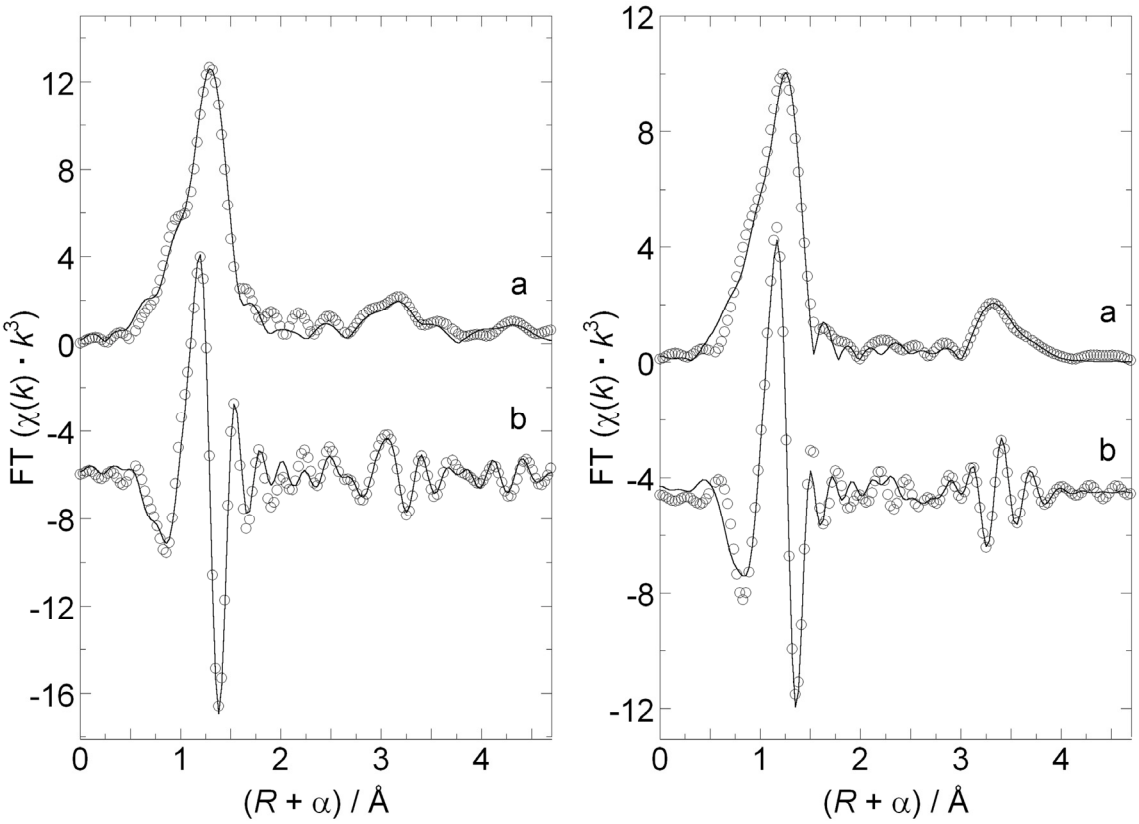

Fig. S12. Left: EXAFS (circles) and curvefit (line) for $MgMoO_4$, using a model that omits the Mo-Mg paths at 3.450 and 3.577 Å, as well as the Mo-Mg-O path at 3.770 Å. Right: EXAFS (circles) and curvefit (line) for $MgMo_2O_7$, using a model that omits the Mo-Mo-O path at 3.748 Å. The FT magnitude (a) and real component (b) are shown. Curvefit parameters can be found in Tables S3 and S4.

Table S4. Comparison of crystal structure-derived distances with the FT EXAFS curvefit parameters[a] for $MgMoO_4$, obtained using a model that omits several key paths

Path	*N*	XRD[1] *d* / Å	EXAFS *R* / Å	Δ*R* Å	σ^2 Å^2
Mo=O	2	1.731	1.734	0.003 ± 0.004	0.0026 ± 0.0002
Mo-O	2	1.800	1.803	0.003 ± 0.004	0.0026 ± 0.0002
Mo-O	2	3.087	3.090	0.003 ± 0.004	0.005 ± 0.003
Mo-O-O	12	3.16-3.35	3.276	0.086 ± 0.07	0.005 ± 0.003
Mo-Mg	0	3.449			
Mo-Mg	0	3.576			
Mo-Mg-O	0	3.770			
Mo-Mo	1	4.078	3.390	-0.69 ± 0.01	0.0019 ± 0.0003
Mo-Mo	1	4.078	3.519	-0.56 ± 0.01	0.0014 ± 0.0004
Mo-O-O	2	4.562	4.535	-0.09 ± 0.04	0.010 ± 0.002
Mo-Mo	4	4.625	4.565	0.003 ± 0.004	0.010 ± 0.002
Mo-Mo	2	4.780	4.783	0.003 ± 0.004	0.010 ± 0.002
Mo-O-O	8	4.790	4.793	0.003 ± 0.004	0.010 ± 0.002

[a] Theoretical paths were generated using Feff 8.20. The number of independent data points is 24.2. Coordination numbers were fixed at their crystal structure values, except for the Mo-Mg and Mo-Mg-O paths at 3.449, 3.576, and 3.770 Å, which were omitted. S_0^2 and ΔE_0 were refined as global parameters, giving (0.99 ± 0.03) and (-7.7 ± 1.0) eV, respectively. Ten other parameters were varied during the fit: five for Δ*R* and five for σ^2.

Table S5. Comparison of crystal structure-derived distances with FT EXAFS curvefit parameters[a] for $MgMo_2O_7$, obtained by omitting a key multiple-scattering path

Path	N	XRD[2] d / Å	EXAFS R / Å	ΔR Å	σ^2 Å^2
Mo=O	2	1.706 - 1.727	1.723	0.003 ± 0.006	0.0034 ± 0.0004
Mo-O	1	1.744 - 1.781	1.747	0.003 ± 0.006	0.006 ± 0.002
Mo-O	1	1.857 - 1.881	1.860	0.003 ± 0.006	0.006 ± 0.002
Mo-O	0.5	2.859	2.844	-0.02 ± 0.04	0.006 ± 0.002
Mo-Mg	0.5	3.374	3.356	-0.02 ± 0.04	0.006 ± 0.002
Mo-O	0.5	3.374	3.359	-0.02 ± 0.04	0.006 ± 0.002
Mo-Mg	1	3.639 - 3.703	3.569	-0.07 ± 0.02	0.002 ± 0.002
Mo-O	0.5	3.664	3.648	-0.02 ± 0.04	0.006 ± 0.002
Mo-Mo	1	3.685	3.815	0.13 ± 0.07	0.009 ± 0.005
Mo-Mo-O	0	3.711			
Mo-O	0.5	3.713	3.698	-0.02 ± 0.04	0.0034 ± 0.0004
Mo-Mg-O	2	3.720	3.704	-0.02 ± 0.04	0.006 ± 0.002
Mo-Mg-O	1	3.746	3.755	0.01 ± 0.07	0.006 ± 0.002
Mo-Mo	1	4.108	4.074	0.39 ± 0.04	0.007 ± 0.004

[a] Theoretical paths were generated for each crystallographically distinct Mo center, using Feff 8.20. The number of independent data points is 24.2. Coordination numbers were fixed at their crystal structure values, except for the Mo-Mo-O path at 3.711 which was omitted. S_0^2 and ΔE_0 were refined as global parameters, giving (0.99 ± 0.03) and (-9.6 ± 1.1) eV, respectively. Eleven other parameters were varied during the fit: six for ΔR and five for σ^2.