XAFS Studies of Nickel and Sulfur Speciation in Residual Oil Fly-Ash Particulate Matters (ROFA PM)

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Summary:

No of Pages: 5

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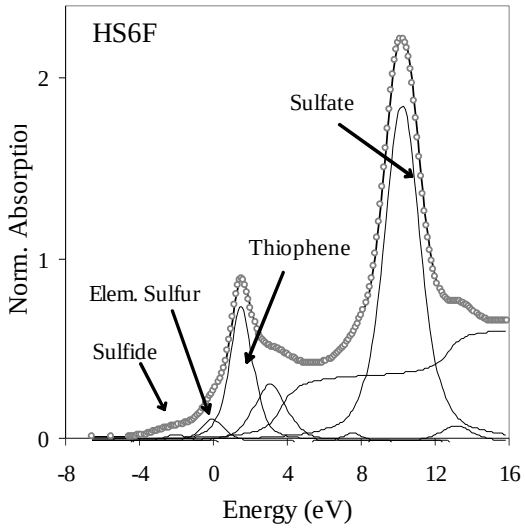

Figure S1. S K-edge XANES spectrum of HS6F (ooo) and the calculated fit (—), deconvoluted individual components (—) are shown underneath the fit.

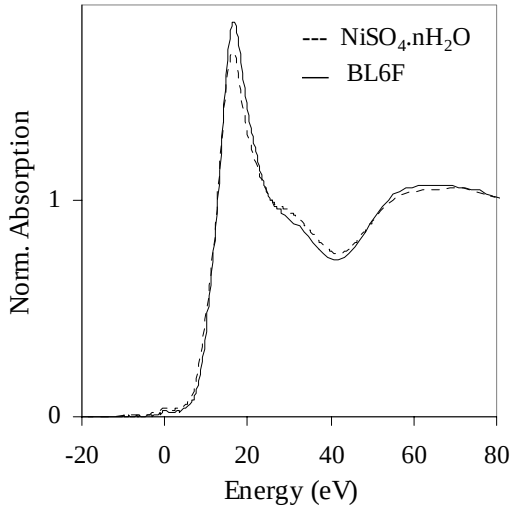

Figure S2. Normalized Ni K-edge XANES spectra of BL6F (—) and $NiSO_4.nH_2O$ (-----).

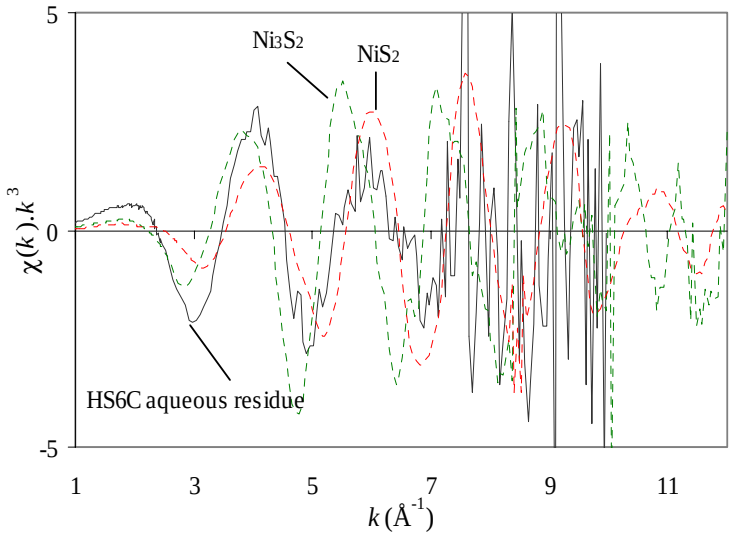

Figure S3. Ni K-edge EXAFS of HS6C residue, Ni_3S_2, and NiS_2.

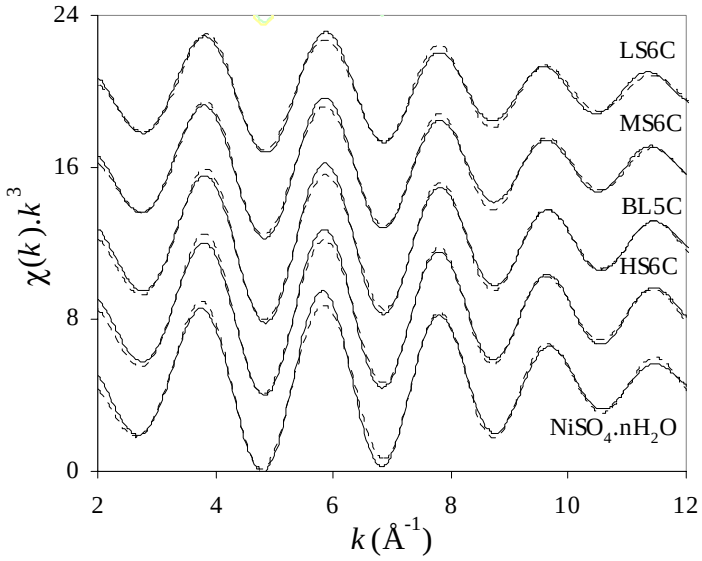

Figure S4. Back-transformed 1st shell Ni-O EXAFS (—) and calculated pattern (---) based on NiO_N model, where the coordination number N was subjected to variation.

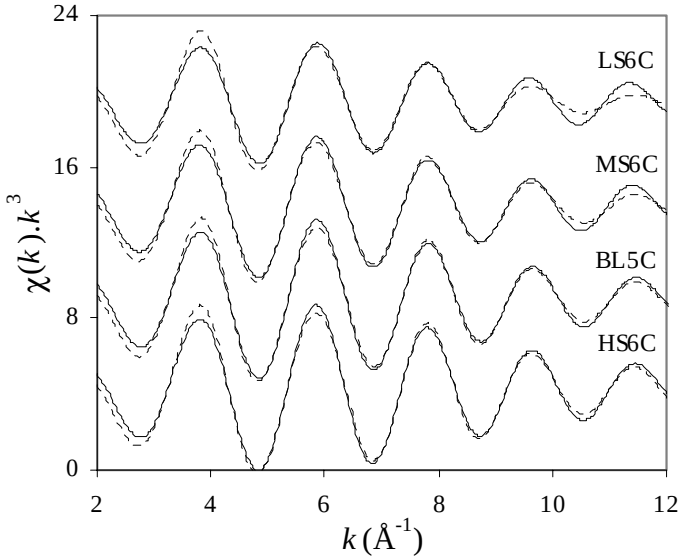

Figure S5. Back-transformed 1st shell Ni-O EXAFS (—) and calculated pattern (---) based on NiO_6 model, where the coordination number was fixed at six.

Table S1. Ni coordination in ROFA $PM_{2.5+}$: distance (d), Debye-Waller factor (σ^2), coordination number (N) and energy shift (ΔE_o).

Sample	shell	d/Å	σ^2/Å^2	N	ΔE_o/eV	Δk/Å^{-1}	*R*
$NiSO_4.nH_2O$	Ni-O	2.05	0.007	6	-3.7	2.0-12.0	9
HS6C	Ni-O	2.06	0.007	6	-1.9	2.0-12.0	11.5
BL5C	Ni-O	2.06	0.008	6	-1.5	2.0-12.0	12.2
MS6C	Ni-O	2.06	0.009	6	-1.8	2.0-12.0	15.1
LS6C	Ni-O	2.07	0.011	6	-1.1	2.0-12.0	20.1

$S_o^2 = 0.9$, *R* – residual factor (in %).

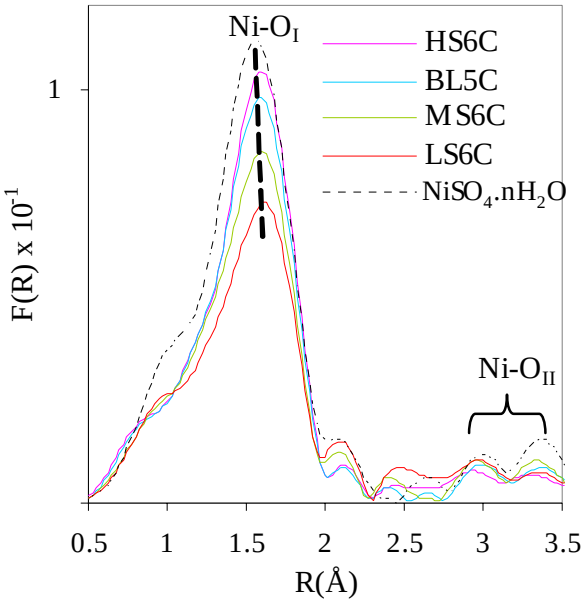

Figure S6. RSF of all four $PM_{2.5+}$ samples from FTB compared with that of $NiSO_4.nH_2O$

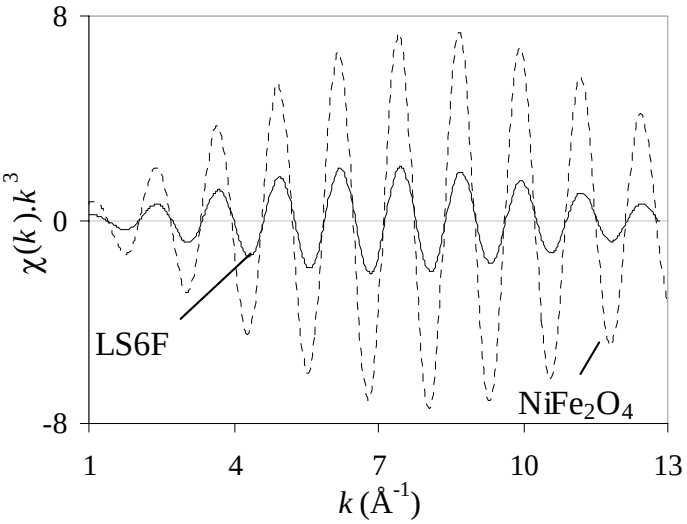

Figure S7. Back-transformed Ni-(Ni/Fe) RSF peak of LS6F compared with that of $NiFe_2O_4$.

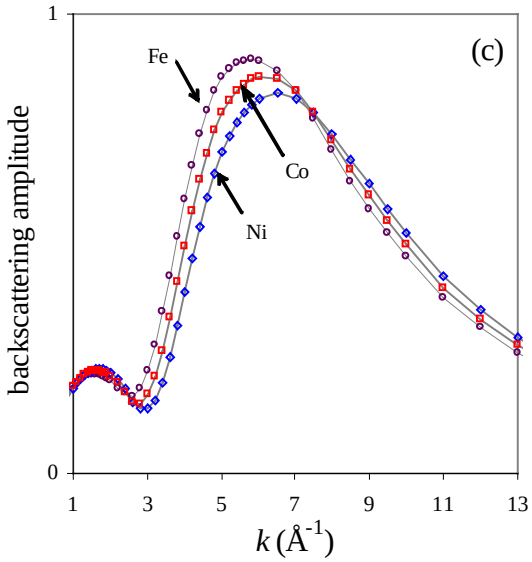

Figure S8. Backscattering amplitudes of Fe, Co, and Ni.