XAS study of Sn speciation in toothpaste

Supplementary Information

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Sn(II)-based compounds	Sn(IV)-based compounds
SnF_2 (solid/aq)	SnO_2
SnF_2 + Carrageenan	$SnCl_4$, $5H_2O$ + NaOH*
SnF_2 + Na-Gluconate*	
SnF_2 + Glycerol*	
$SnCl_2$ + Na-Acetate	
$SnCl_2$ + NaCl	
$SnCl_2$ + Na-Gluconate	
$SnCl_2$ + NaF	
SnF_2 + NaF	
SnF_2 + Mica	
SnF_2 + NaF*	
SnF_2 + Na_3PO_4	
SnF_2 + Polyphosphate	
SnF_2 + TiO_2	
SnF_2 + Zn-Lactate	
SnO	* = various ratio analyzed
$Sn_2P_2O_7$	= select references (XANES)
SnF_2 + Na_2HPO_4*	= select references (EXAFS)
SnF_2 + $Na_4P_2O_7$	

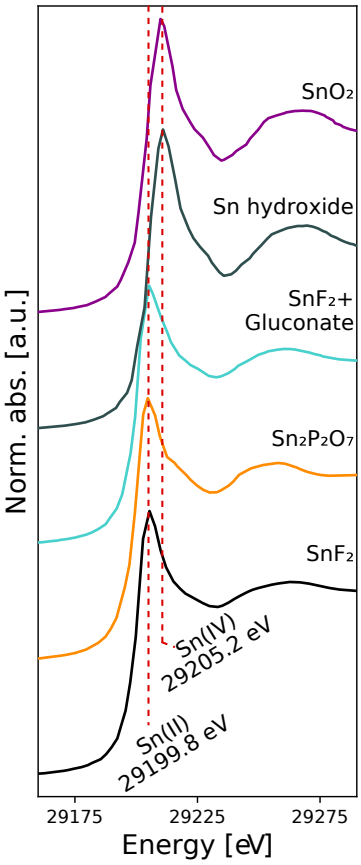

Figure S1: Sn(II)- and Sn(IV)-based compounds measured and analyzed as references for Sn K-edge XANES and EXAFS data analysis. XANES spectra of some of those compounds is also presented, with the mean whiteline values for Sn(II) and Sn(IV) compounds.

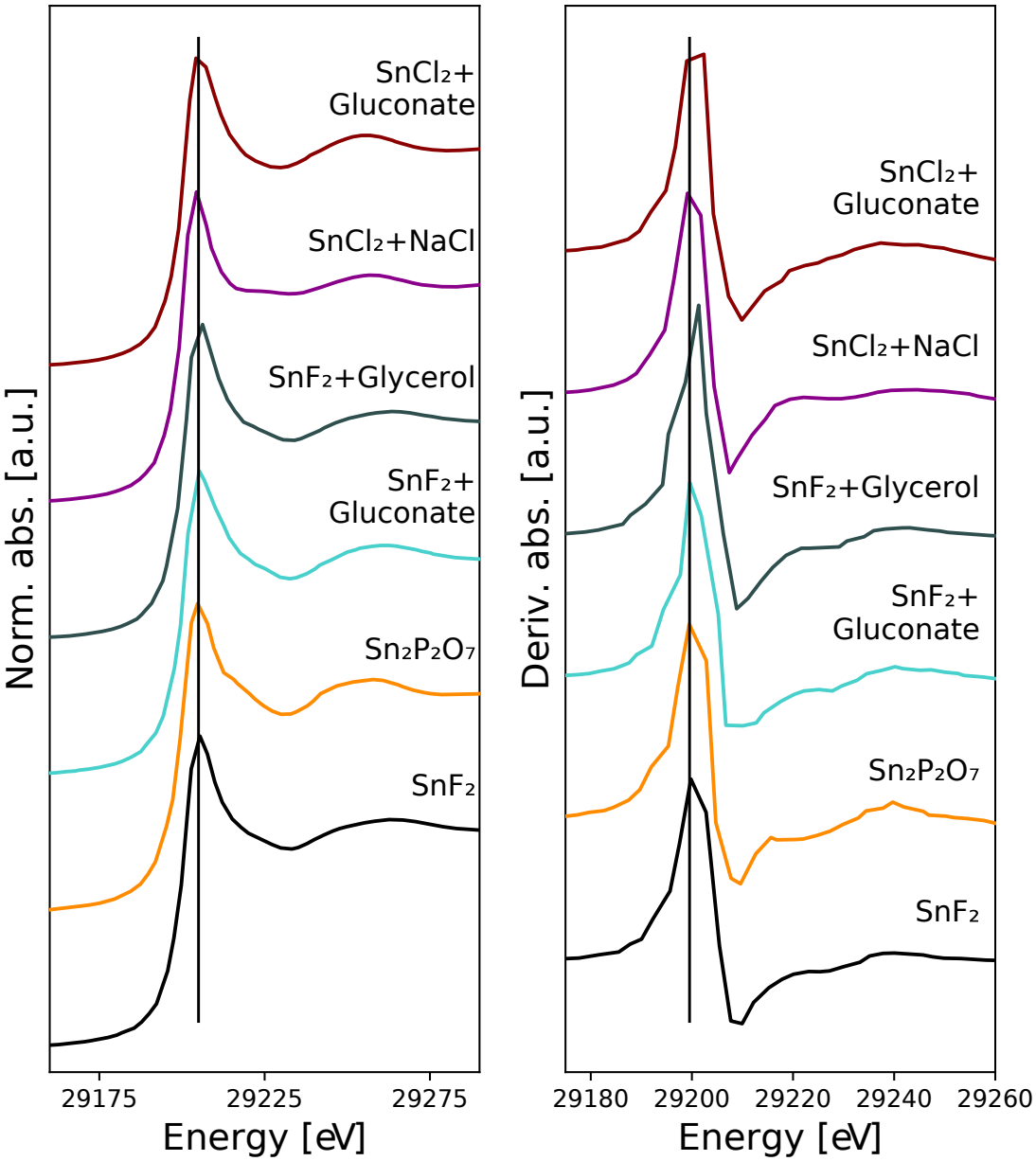

Figure S2: Sn K-edge XANES and First Derivate XANES spectra of Sn(II)-based compounds.

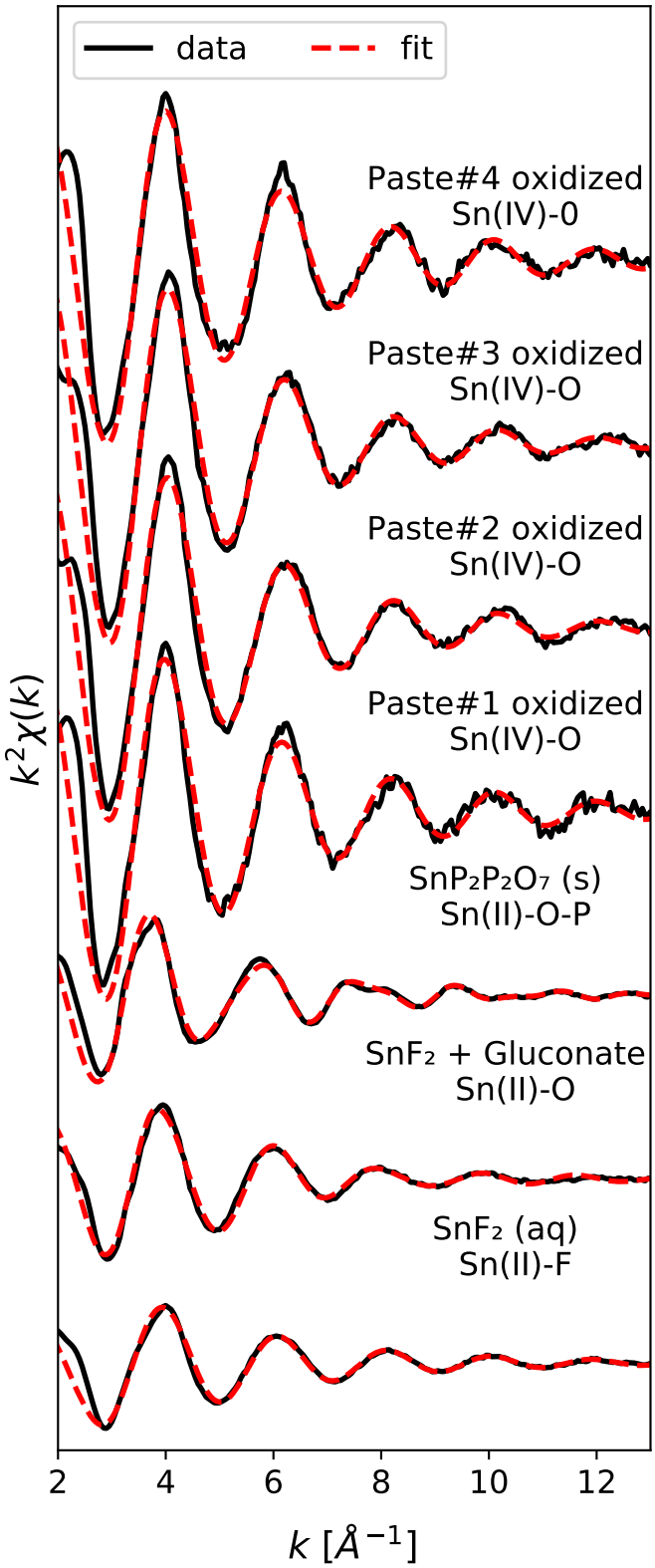

Figure S3: Results of least-squares fitting (LSF) analysis on Sn K-edge EXAFS spectra reference compounds.

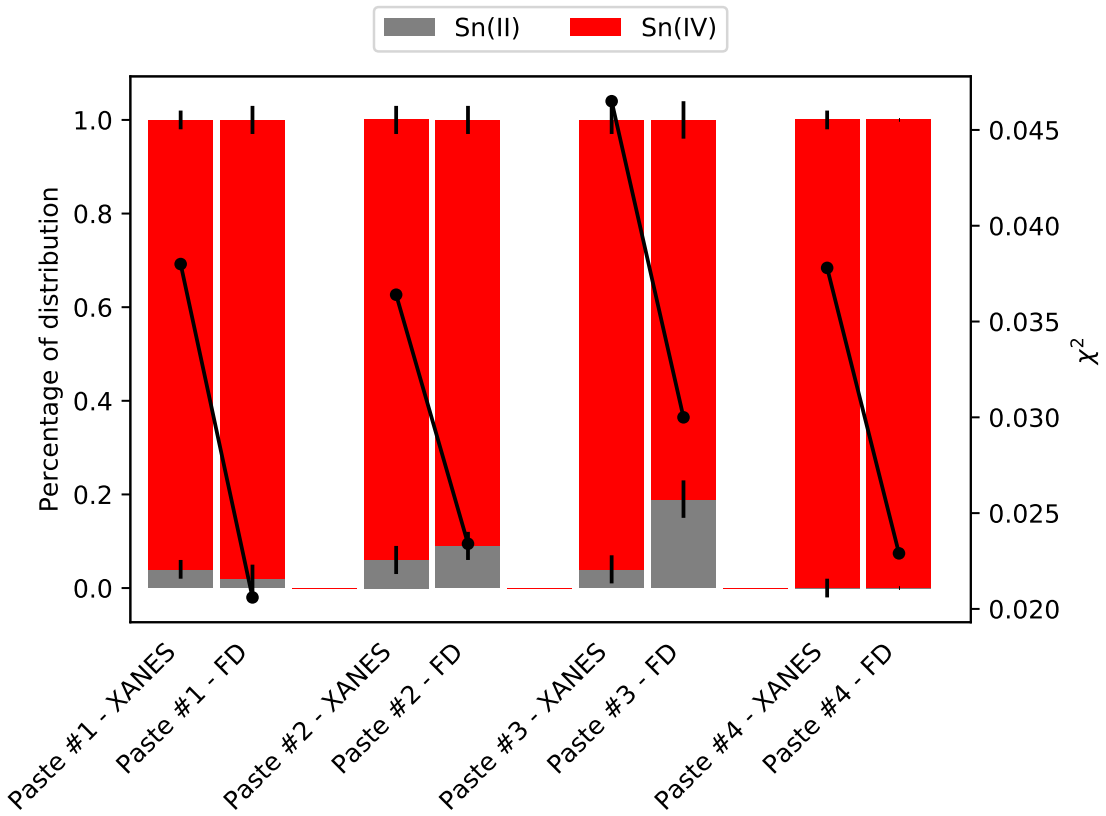

Figure S4: Results of Linear Combination Fit for the pastes oxidized, obtained by fitting the XANES and First-Derivative (FD) experimental data.

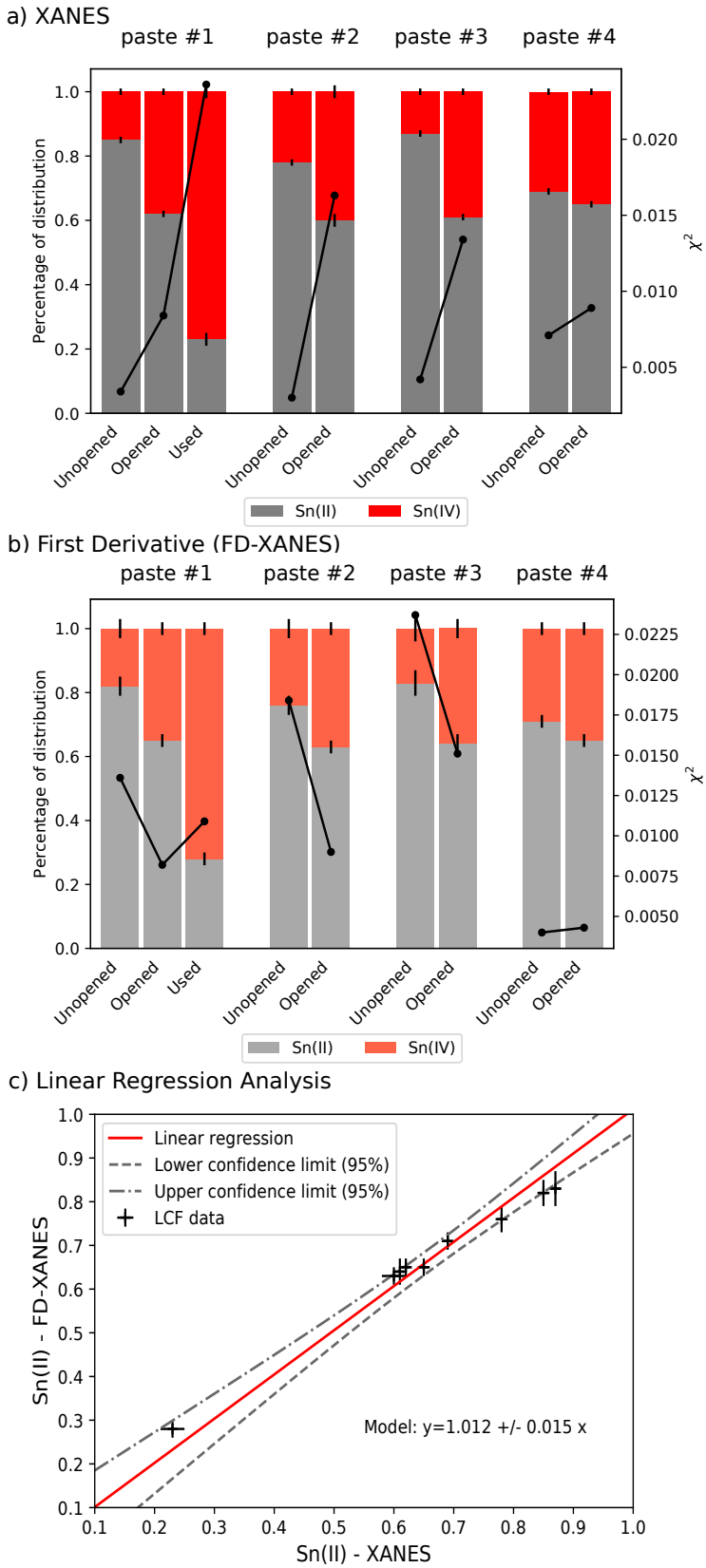

Figure S5: Results of Linear Combination Fit for XANES and XANES-FD spectra as well as the correlation between the results.

Table S1: Chemical Suppliers of the compounds used in this study

Compound	Supplier	Purity (%)	Origin
SnF_2	Aldrich	99	USA
$SnCl_2, 2H_2O$	Alfa Aesar	99	USA
$SnCl_4, 5H_2O$	Acros	98+	India
$Sn_2P_2O_7$	Aldrich	98	USA
SnO_2	Alfa Aesar	99.9	USA
SnO	Aldrich	97	USA
$Na - Acetate$	Merck	99+	Germany
NaCl	Fisher Chemicals	99.9	USA
$Na - Gluconate$	Sigma	99	France
NaF	Fisher Scientific	99	USA
$Na_3PO_4, 5H_2O$	Sigma	98+	Germany
$Na_5P_3O_{10}$	Alfa Aesar	98	USA
Na_2HPO_4	Sigma	99	Japan
$Na_2P_2O_7, 10H_2O$	Sigma-Aldrich	98	USA
$Zn - Lactate$	Colgate		USA
TiO_2	Colgate		USA
Mica	Colgate		USA
Carrageenan	Colgate		USA
Glycerol	Sigma	99	Malaysia

Table S2: Part of the compounds present in the four toothpastes analyzed

Compound	Paste #1	Paste#2	Paste#3	Paste#4
Glycerin	*		*	*
Water	*	*	*	
Sorbitol	*	*		
Hydrated Silica	*	*	*	*
Stannous Chloride		*	*	
Trisodium phosphate			*	
Sodium hexametaphosphate			*	
Pentasodium triphophaste				*
Tetrasodium pyrophosphate	*			
Zinc phosphate	*			
Sodium Gluconate		*	*	
Polyacrylic Acid				*
Sodium Citrate	*			
Cocamidopropyl Betaine				*