

Hedman  
Pianetta

X-RAY ABSORPTION  
FINE STRUCTURE



882

AIP

ISBN 978-0-7354-0384-0  
ISSN 0094-243X

# X-RAY ABSORPTION FINE STRUCTURE—XAFS13

13<sup>th</sup> International Conference

Stanford, California, U.S.A. 9 - 14 July 2006



EDITORS  
Britt Hedman  
Piero Pianetta

AMERICAN  
INSTITUTE  
OF PHYSICS

AIP CONFERENCE PROCEEDINGS ■ 882

X-RAY ABSORPTION

FINE STRUCTURE—XAFS13

To learn more about the AIP Conference Proceedings, including the  
Conference Proceedings Series, please visit the webpage  
**<http://proceedings.aip.org/proceedings>**

# X-RAY ABSORPTION FINE STRUCTURE—XAFS13

13<sup>th</sup> International Conference

Stanford, California, U.S.A. 9 - 14 July 2006



*EDITORS*

Britt Hedman

Piero Pianetta

*Stanford Synchrotron Radiation Laboratory*

*Stanford, California, U.S.A.*

**SPONSORING ORGANIZATION**

International XAFS Society

**AMERICAN  
INSTITUTE  
OF PHYSICS**

Melville, New York, 2007

AIP CONFERENCE PROCEEDINGS ■ VOLUME 882

## **Editors**

Britt Hedman  
Piero Pianetta

Stanford Synchrotron Radiation Laboratory  
Stanford Linear Accelerator Center  
Stanford University  
2575 Sand Hill Road, MS69  
Menlo Park, CA 94025, USA

E-mail: [hedman@ssrl.slac.stanford.edu](mailto:hedman@ssrl.slac.stanford.edu)  
[pianetta@stanford.edu](mailto:pianetta@stanford.edu)

Authorization to photocopy items for internal or personal use, beyond the free copying permitted under the 1978 U.S. Copyright Law (see statement below), is granted by the American Institute of Physics for users registered with the Copyright Clearance Center (CCC) Transactional Reporting Service, provided that the base fee of \$23.00 per copy is paid directly to CCC, 222 Rosewood Drive, Danvers, MA 01923. For those organizations that have been granted a photocopy license by CCC, a separate system of payment has been arranged. The fee code for users of the Transactional Reporting Services is: ISBN/978-0-7354-0384-0/07/\$23.00.

© 2007 American Institute of Physics

Permission is granted to quote from the AIP Conference Proceedings with the customary acknowledgment of the source. Republication of an article or portions thereof (e.g., extensive excerpts, figures, tables, etc.) in original form or in translation, as well as other types of reuse (e.g., in course packs) require formal permission from AIP and may be subject to fees. As a courtesy, the author of the original proceedings article should be informed of any request for republication/reuse. Permission may be obtained online using Rightslink. Locate the article online at <http://proceedings.aip.org>, then simply click on the Rightslink icon/"Permission for Reuse" link found in the article abstract. You may also address requests to: AIP Office of Rights and Permissions, Suite 1N01, 2 Huntington Quadrangle, Melville, NY 11747-4502; Fax: 516-576-2450; Tel.: 516-576-2268; E-mail: [rights@aip.org](mailto:rights@aip.org).

L.C. Catalog Card No. 2006939767  
ISBN 978-0-7354-0384-0  
ISSN 0094-243X

Printed in the United States of America

## CONTENTS

<b>Preface</b> .....	<b>xix</b>
<b>Conference Committees</b> .....	<b>xx</b>
<b>XAFS13 Conference Overview</b> .....	<b>xxi</b>
G. E. Brown, Jr.	

## DALE SAYERS SYMPOSIUM

<b>Dale Sayers Festschrift</b> .....	<b>3</b>
E. A. Stern	
<b>Dale Sayers' Scientific Legacy in North Carolina</b> .....	<b>10</b>
M. A. Paesler and J. S. Washington	
<b>The Ferritin Protein Nanocage and Biomineral, from Single Fe Atoms to FeO Nanoparticles: Starting with EXAFS.</b> .....	<b>15</b>
E. C. Theil	
<b>Local Bonding Arrangements in Ge<sub>2</sub>Sb<sub>2</sub>Te<sub>5</sub>: Importance of Ge and Te Bonding in Optical Memory Materials</b> .....	<b>19</b>
D. A. Baker	
<b>Ultrafast XAFS Measurements on Laser Excited Ge Films.</b> .....	<b>24</b>
E. A. Stern and D. Brewes	

## PLENARY

<b>Capturing Transient Electronic and Molecular Structures in Liquids by Picosecond X-ray Absorption Spectroscopy.</b> .....	<b>31</b>
W. Gawelda, V. T. Pham, A. El Nahhas, M. Kaiser, Y. Zaushitsyn, S. L. Johnson, D. Grolimund, R. Abela, A. Hauser, C. Bressler, and M. Chergui	
<b>Novel Techniques and Approaches to Unravel the Nature of X-ray Absorption Spectra</b> .....	<b>37</b>
F. M. F. de Groot	
<b>Durability of Silicate Glasses: An Historical Approach</b> .....	<b>44</b>
F. Farges, M.-P. Etcheverry, A. Haddi, P. Trocellier, E. Curti, and G. E. Brown, Jr.	
<b>XANES in Nanobiology</b> .....	<b>51</b>
R. A. Metzler, R. M. Olabisi, M. Abrecht, D. Ariosa, C. J. Johnson, B. Gilbert, B. H. Frazer, S. N. Coppersmith, and P. U. P. A. Gilbert	

## THEORY AND MODELING

<b>What Can We Learn from a Detailed Study of the Temperature Dependence of <math>\sigma</math>, the Width of the Pair Distribution Function?</b> .....	<b>59</b>
F. Bridges, L. Downward, Y. Jiang, and T. O'Brien	
<b>Local Structure in Solid Solutions Revealed by Combined XAFS/Neutron PD Refinement, Using the Multiple-scattering RMC Method</b> .....	<b>64</b>
N. Binsted, C. Owens, and M. T. Weller	
<b>Bayes-Turchin Analysis of Overlapping L-Edges EXAFS Data of Iron</b> .....	<b>69</b>
H. H. Rossner, D. Schmitz, P. Imperia, H. J. Krappe, and J. J. Rehr	
<b>Improving Resolution in k and r Space: A FEFF-based Wavelet for EXAFS Data Analysis</b> .....	<b>72</b>
H. Funke, M. Chukalina, A. Voegelin, and A. C. Scheinost	
<b>Theory of Optical Field Effects in XAFS</b> .....	<b>75</b>
T. Fujikawa and H. Arai	
<b>XMCD Analysis beyond Standard Procedures</b> .....	<b>78</b>
H. Wende, A. Scherz, C. Sorg, K. Baberschke, E. K. U. Gross, H. Appel, K. Burke, J. Minár, H. Ebert, A. L. Ankudinov, and J. J. Rehr	
<b>New Approach for 3D Local Structure Refinement Using Non-Muffin-Tin XANES Analysis</b> .....	<b>83</b>
G. Smolentsev, A. V. Soldatov, and M. C. Feiters	

<b>Inelastic Losses and Multi-electron Excitations in X-ray Spectra</b> .....	<b>85</b>
J. J. Rehr, J. J. Kas, M. P. Prange, A. P. Sorini, L. W. Campbell, and F. D. Vila	
<b>Study of the Electronic Structure in Oxides Using Absorption and Resonant X-ray Scattering</b> .....	<b>89</b>
Y. Joly, E. Nazarenko, E. Lorenzo, S. Di Matteo, and C. R. Natoli	
<b>Advances in EXAFS Studies of Thermal Properties of Crystals</b> .....	<b>94</b>
P. Fornasini	
<b>Cu <math>K\alpha</math> X-ray Emission Spectroscopy in <math>\text{La}_2\text{CuO}_4</math></b> .....	<b>99</b>
A. Kotani, K. Okada, M. Calandra, and A. Shukla	
<b>Recent Developments in the Analysis of X-ray Raman Scattering</b> .....	<b>102</b>
J. A. Soininen, J. J. Rehr, A. Mattila, S. Galambosi, and K. Hämäläinen	
<b>PySpline: A Modern, Cross-platform Program for the Processing of Raw Averaged XAS Edge and EXAFS Data</b> .....	<b>105</b>
A. Tenderholt, B. Hedman, and K. O. Hodgson	
<b>Theory of Electron-phonon Interaction in XAFS and Other Spectroscopies</b> .....	<b>108</b>
H. Arai, N. Ueno, and T. Fujikawa	
<b>Progresses in the MXAN Fitting Procedure</b> .....	<b>111</b>
K. Hayakawa, K. Hatada, S. D. Longa, P. D'Angelo, and M. Benfatto	
<b>Multiple Scattering Approach to Continuum State with Generally Shaped Potential</b> .....	<b>114</b>
K. Hatada, K. Hayakawa, A. Tenore, M. Benfatto, and C. Natoli	
<b>Non-MT Determination of X-ray Absorption Cross Section's Factorized Atomic Part in the Near-edge Region. Application to Si K-Edge XANES Analysis in Beta-Zeolites</b> .....	<b>117</b>
L. A. Bugaev, J. A. van Bokhoven, L. A. Avakyan, and Y. V. Latokha	
<b>Ti <math>K</math> Pre-Edge in <math>\text{SrTiO}_3</math> under Pressure: Experiments and Full-potential First-principles Calculations</b> .....	<b>120</b>
D. Cabaret, B. Couzinet, A.-M. Flank, J.-P. Itié, P. Lagarde, and A. Polian	
<b>New Developments in Charge Transfer Multiplet Calculations: Projection Operations, Mixed-spin States and <math>\pi</math>-Bonding</b> .....	<b>123</b>
F. M. F. de Groot, R. K. Hocking, C. Piamonteze, B. Hedman, K. O. Hodgson, and E. I. Solomon	
<b><i>Ab Initio</i> Calculation of XAFS Debye-Waller Factors for Crystalline Materials</b> .....	<b>126</b>
N. Dimakis	
<b>A Variation of the F-Test for Determining Statistical Relevance of Particular Parameters in EXAFS Fits</b> .....	<b>129</b>
L. Downward, C. H. Booth, W. W. Lukens, and F. Bridges	
<b>EXAFS Energy Shift and Structural Parameters</b> .....	<b>132</b>
S. D. Kelly and B. Ravel	
<b>EXAFS Analysis with Self-consistent Atomic Potentials</b> .....	<b>135</b>
S. D. Kelly and B. Ravel	
<b>Self-consistent EXAFS PDF Projection Method by Matched Correction of Fourier Filter Signal Distortion</b> .....	<b>138</b>
J. M. Lee and D.-S. Yang	
<b>An Abnormally Large EXAFS Debye-Waller Factor for a Mo-O Bond in Hexamolybdate</b> .....	<b>141</b>
S. Furuta, T. Miyayaga, and I. Watanabe	
<b>The Beta Environmental Fine Structure (BEFS): The XAFS Nuclear Analogue</b> .....	<b>144</b>
A. Monfardini, G. Benedek, O. Cremonesi, A. Filippini, A. Nucciotti, and M. Sisti	
<b>Relativistic Multiple Scattering Approach to Heavy Metal <math>L_{2,3}</math>-Edge XMCD</b> .....	<b>147</b>
K. Okamoto, S. Nagamatsu, T. Fujikawa, and H. Maruyama	
<b>The Difficult Chore of Measuring Coordination by EXAFS</b> .....	<b>150</b>
B. Ravel and S. D. Kelly	
<b>New Regularization Method for EXAFS Analysis</b> .....	<b>153</b>
T. Y. Reich, M. E. Korshunov, T. V. Antonova, A. L. Ageev, H. Moll, and T. Reich	
<b>Measurement of the Full XAFS Spectrum of MgO Using Nonresonant Inelastic X-ray Scattering</b> .....	<b>156</b>
T. T. Fister, G. T. Seidler, J. O. Cross, J. J. Rehr, and J. A. Soininen	
<b>XMCD Spectra of Co Clusters on Au(111) by <i>Ab-Initio</i> Calculations</b> .....	<b>159</b>
O. Šípr, J. Minár, S. Bornemann, and H. Ebert	
<b>REX2000 Version 2.5: Improved DATA Handling and Enhanced User Interface</b> .....	<b>162</b>
T. Taguchi	

<b>Solving a Historical Puzzle</b> .....	165
M. Groves, E. A. Stern, G. Seidler, and M. Balasubramanian	
<b>The First and Second Shell Correlation Analysis in Cu Metal by the Matched EXAFS PDF Projection Method</b> .....	168
D.-S. Yang and J. M. Lee	

## ENVIRONMENTAL AND EARTH SCIENCES

<b>XAFS Study of the Chemical and Structural States of Technetium in Fe(III) Oxide Co-precipitates</b> .....	173
S. M. Heald, J. M. Zachara, B.-H. Jeon, J. P. McKinley, R. Kukkadapu, and D. Moore	
<b>Speciation of Iron in Atmospheric Particulate Matter by EXAFS</b> .....	176
W. Yinsong, L. Aiguo, Z. Yuanxun, X. Yaning, L. Delu, L. Yan, and Z. Guilin	
<b>Application of XAFS Spectroscopy to Actinide Environmental Science</b> .....	179
T. Reich, T. Y. Reich, S. Amayri, J. Drebert, N. L. Banik, R. A. Buda, J. V. Kratz, and N. Trautmann	
<b>Molecular Characterization of Actinide Oxocations from Protactinium to Plutonium</b> .....	184
C. Den Auwer, P. Guilbaud, D. Guillaumont, P. Moisy, V. Digandomenico, C. Le Naour, D. Trubert, E. Simoni, C. Hennig, A. Scheinost, and S. D. Conradson	
<b>Confocal <math>\mu</math>-XRF, <math>\mu</math>-XAFS, and <math>\mu</math>-XRD Studies of Sediment from a Nuclear Waste Disposal Natural Analogue Site and Fractured Granite Following a Radiotracer Migration Experiment</b> .....	187
M. A. Denecke, K. Janssens, B. Brendebach, W. De Nolf, G. Falkenberg, J. Rothe, R. Simon, A. Somogyi, B. Vekemans, and U. Noseck	
<b>Micro-scale Heterogeneity in Biogeochemical Uranium Cycling</b> .....	190
M. Ginder-Vogel, W.-M. Wu, S. Kelly, C. S. Criddle, J. Carley, P. Jardine, K. M. Kemner, and S. Fendorf	
<b>Understanding Humic Acid/Zr(IV) Interaction—A Spectromicroscopy Approach</b> .....	193
J. Rothe, M. Plaschke, and M. A. Denecke	
<b>XAFS Determination of Pb and Cd Speciation with Siderophores and the Metal/Siderophore/Kaolinite System</b> .....	196
B. Mishra, E. A. Haack, I. F. Vasconcelos, P. A. Maurice, and B. A. Bunker	
<b>Environmental Impact of Steel Slag Reused as Aggregates in Road Manufacturing: Molecular Mechanisms of Chromium and Vanadium Release</b> .....	199
P. Chaurand, J. Rose, O. Proux, J. L. Hazemann, V. Briois, M. Salome, J. Susini, J. H. Ferrasse, D. Borschneck, and J. Y. Bottero	
<b>A pH-dependent X-ray Absorption Spectroscopy Study of U Adsorption to Bacterial Cell Walls</b> .....	202
B. Ravel, S. D. Kelly, D. Gorman-Lewis, M. I. Boyanov, J. B. Fein, and K. M. Kemner	
<b>Extended vs. Local Structure in Sb-Pyrochlores: An Illustration of the Valuable Interplay between Crystallography and XAFS</b> .....	205
M.-O. Figueiredo	
<b>Coordination Environments of Highly Charged Cations (Ti, Cr, and Light REE's) in Borosilicate Glass/Melts to 1120°C</b> .....	208
F. Farges and G. E. Brown, Jr.	
<b>XAS Studies of Arsenic in the Environment</b> .....	211
J. M. Charnock, D. A. Polya, A. G. Gault, and A. J. Morgan	
<b>Local Structures around Si, Al and Na in Hydrated Silicate Glasses</b> .....	214
F. Farges, S. de Wispelaere, S. Rossano, M. Muños, M. Wilke, A.-M. Flank, and P. Lagarde	
<b>Adsorption Mechanisms of Trivalent Gold onto Iron Oxy-Hydroxides: From the Molecular Scale to the Model</b> .....	217
B. Cancès, M. Benedetti, F. Farges, and G. E. Brown, Jr.	
<b>Discovery of Unusual Minerals in Paleolithic Black Pigments from Lascaux (France) and Ekain (Spain)</b> .....	220
E. Chalmin, F. Farges, C. Vignaud, J. Susini, M. Menu, and G. E. Brown, Jr.	
<b>Chrysocolla Redefined as Spertiniite</b> .....	223
F. Farges, K. Benzerara, and G. E. Brown, Jr.	
<b>Mg K-Edge XANES Spectra in Crystals and Oxide Glasses: Experimental vs. Theoretical Approaches</b> .....	226
N. Trcera, D. Cabaret, F. Farges, A.-M. Flank, P. Lagarde, and S. Rossano	



<b>Selenium Speciation in Biofilms from Granular Sludge Bed Reactors Used for Wastewater Treatment</b> .....	229
E. van Hullenbusch, F. Farges, M. Lenz, P. Lens, and G. E. Brown, Jr.	
<b>Speciation of Phosphate in Iron Rich Mineral Deposit in a High Mountain Lake Environment, a Study at the Micron Scale at the LUCIA Beamline</b> .....	232
D. Vantelon, A. Hofmann, K. Hanselmann, and A.-M. Flank	
<b>Local Structure of Transition Elements (V, Cr, Mn, Fe and Zn) in Al<sub>2</sub>SiO<sub>5</sub> Polymorphs</b> .....	235
Y. Furukawa, A. Yoshiasa, H. Arima, M. Okube, K. Murai, and T. Nishiyama	
<b>Adsorption and Precipitation of Aqueous Zn(II) on Hematite Nano- and Microparticles</b> .....	238
J. Ha, F. Farges, and G. E. Brown, Jr.	
<b>High Pressure XAS at the Ti K Edge on Titanate Perovskites</b> .....	241
J. P. Itié, B. Couzinet, A.-M. Flank, P. Lagarde, and A. Polian	
<b>XAFS of Synthetic Iron(III)-Arsenate Co-precipitates and Uranium Mill Neutralized Raffinate</b> .....	244
N. Chen, D. T. Jiang, J. Cutler, G. P. Demopoulos, and J. W. Rowson	
<b>EXAFS Signatures of Structural Zn at Trace Levels in Layered Minerals</b> .....	247
F. Juillot, G. Morin, J.-L. Hazemann, O. Proux, S. Belin, V. Briois, G. E. Brown, Jr., and G. Calas	
<b>XAFS and X-ray and Electron Microscopy Investigations of Radionuclide Transformations at the Mineral-microbe Interface</b> .....	250
K. Kemner, E. O'Loughlin, S. Kelly, B. Ravel, M. I. Boyanov, D. Sholto-Douglas, B. Lai, R. Cook, E. E. Carpenter, V. Harris, and K. Nealson	
<b>Local Structure around Iron Ions in Anatase TiO<sub>2</sub></b> .....	253
S. Zhu, W. Liu, S. Wei, C. Fan, and Y. Li	
<b>On the Coordination of Actinides and Fission Products in Silicate Glasses</b> .....	256
A. Haddi, F. Farges, P. Trocellier, E. Curti, M. Harfouche, and G. E. Brown, Jr.	
<b>Redox and Speciation of Uranium in Al-rich Perovskites from High-pressure/High-temperature Conditions</b> .....	259
S. Greaux, F. Farges, L. Gautron, I. Letard, A.-M. Flank, and P. Lagarde	
<b>The Structure of Uranyl Sulfate in Aqueous Solution—Monodentate versus Bidentate Coordination</b> .....	262
C. Hennig, K. Schmeide, V. Brendler, H. Moll, S. Tsushima, and A. C. Scheinost	
<b>EXAFS Study of Filled Skutterudites PrOs<sub>4</sub>Sb<sub>12</sub> and LaOs<sub>4</sub>Sb<sub>12</sub></b> .....	265
K. Nitta, D. Kikuchi, T. Miyanaaga, K. Takegahara, H. Sugawara, and H. Sato	
<b>Speciation of Heavy Metals in Katrina Sediments from New Orleans, Louisiana</b> .....	268
A. Roy, C. Bianchetti, R. Tittsworth, and J. Pardue	
<b>X-ray Absorption Fine Structure Spectroscopy Study of Arsenate Adsorption on Schwertmannite</b> .....	271
M. Sakamaki, H. Takahashi, T. Konishi, A. Inoue, and T. Fujikawa	
<b>XAFS Study of As in K-T Boundary Clays</b> .....	274
S. Sakai, A. Yoshiasa, H. Arima, M. Okube, C. Numako, and T. Sato	
<b>Biogenic UO<sub>2</sub>—Characterization and Surface Reactivity</b> .....	277
D. M. Singer, F. Farges, and G. E. Brown, Jr.	
<b>Chemical Speciation of Chromium in Drilling Muds</b> .....	280
T. Taguchi, M. Yoshii, and K. Shinoda	
<b>Determination of Chemical States of Mercury on Activated Carbon Using XANES</b> .....	283
M. Takaoka, T. Yamamoto, N. Takeda, K. Oshita, T. Tanaka, and T. Uruga	
<b>Chemical Structure of Copper in Incineration Dry Scrubber and Bag Filter Ashes</b> .....	286
M. C. Hsiao, H. P. Wang, C. Y. Peng, C. H. Huang, and Y.-L. Wei	
<b>Local Structures around Co Atoms in Wurtzite ZnO Nano-composites Probed by Fluorescence XAFS</b> .....	289
T. Shi, W. Liu, and S. Wei	
<b>Redox Reaction in Silicate Melts Monitored by “Static” <i>In-Situ</i> Fe K-Edge XANES up to 1180° C</b> .....	293
M. Wilke, G. M. Partzsch, E. Welter, and F. Farges	
<b>Local Structure Analysis around Kr in Minerals by XAFS</b> .....	296
M. Okube, A. Yoshiasa, T. Matsumoto, E. Ito, and Y. Terada	

## BIOLOGICAL AND MEDICAL

<b>Photosynthetic Dioxygen Formation Monitored by Time-resolved X-ray Spectroscopy</b> . . . . .	<b>301</b>
M. Haumann and H. Dau	
<b>Hemeproteins: Recent Advances in Quantitative XANES Analysis</b> . . . . .	<b>306</b>
A. Arcovito, M. Benfatto, P. D'Angelo, and S. Della Longa	
<b>X-ray Absorption Spectroscopy Imaging of Biological Tissues</b> . . . . .	<b>311</b>
I. J. Pickering and G. N. George	
<b>Electronic Structure of the Mn<sub>4</sub>Ca Cluster in the Oxygen-evolving Complex of Photosystem II Studied by Resonant Inelastic X-ray Scattering.</b> . . . . .	<b>316</b>
J. Yano, Y. Pushkar, J. Messinger, U. Bergmann, P. Glatzel, and V. K. Yachandra	
<b>XAS Characterization of the Zn Site of Non-structural Protein 3 (NS3) from Hepatitis C Virus</b> . . . . .	<b>319</b>
I. Ascone, G. Nobili, M. Benfatto, and A. Congiu-Castellano	
<b>Towards a Black-Box for Biological EXAFS Data—I. Identification of Zinc Finger Proteins</b> . . . . .	<b>322</b>
G. Wellenreuther and W. Meyer-Klaucke	
<b>Pharmaceutical Compounds Studied Using NEXAFS</b> . . . . .	<b>325</b>
A. Murray Booth, S. Braun, T. Lonsborough, J. Purton, S. Patel, and S. L. M. Schroeder	
<b>Using XAS and SXRF to Study Copper in Wilson Disease at the Molecular and Tissue Level.</b> . . . . .	<b>328</b>
M. Ralle, N. J. Blackburn, and S. Lutsenko	
<b>First-principles Full-potential Calculations of the Fe K Pre-edge and Near-edge Structure in Carbonmonoxy-Myoglobin</b> . . . . .	<b>331</b>
M. Arfaoui, D. Cabaret, S. Della Longa, A. Seitsonen, and F. Mauri	
<b>XAFS Debye-Waller Factors Temperature-dependent Expressions for Fe<sup>+2</sup>-Porphyrin Complexes</b> . . . . .	<b>334</b>
N. Dimakis and G. Bunker	
<b>EXAFS Studies of Cobalt(II) Complexes with Amino Acids</b> . . . . .	<b>337</b>
S. K. Joshi, V. K. Hinge, and B. D. Shrivastava	
<b>Host-guest Interaction in <math>\alpha</math>-Cyclodextrin Inclusion Complexes</b> . . . . .	<b>340</b>
T. Kaneko, H. Takahashi, K. Ohminami, T. Konishi, M. Ueda, S. Nagamatsu, and T. Fujikawa	
<b>Comparison of Cd Binding Mechanisms by Gram-positive, Gram-negative and Consortia of Bacteria Using XAFS.</b> . . . . .	<b>343</b>
B. Mishra, J. B. Fein, M. I. Boyanov, S. D. Kelly, K. M. Kemner, and B. A. Bunker	
<b>Polarized Range-extended X-ray Absorption Spectroscopy of Oriented Photosystem II Membranes in the S<sub>1</sub> State</b> . . . . .	<b>346</b>
Y. Pushkar, J. Yano, P. Glatzel, J. Messinger, A. Lewis, K. Sauer, U. Bergmann, and V. K. Yachandra	
<b>Valence-to-Core X-ray Emission Spectroscopy as a Tool for Investigation of Organometallic Systems</b> . . . . .	<b>349</b>
G. Smolentsev, A. V. Soldatov, J. Messinger, K. Merz, T. Weyhermuller, Y. Pushkar, J. Yano, V. K. Yachandra, and P. Glatzel	
<b>XAFS Studies of Transition Metal and Halogen Biomaterials in Invertebrate Tools.</b> . . . . .	<b>352</b>
Y. Tao, J. E. Shokes, R. A. Scott, M. H. Nesson, and R. M. S. Schofield	
<b>XAFS Study of the Ferro- and Antiferromagnetic Binuclear Copper(II) Complexes of Azomethine Based Tridentate Ligands</b> . . . . .	<b>355</b>
V. G. Vlasenko, I. S. Vasilchenko, I. V. Pirog, T. E. Shestakova, A. I. Uraev, A. S. Burlov, and A. D. Garnovskii	

## MATERIALS AND MAGNETISM

<b>The Checkerboard Pattern of the Charge-ordered Phases in Bi<sub>1-x</sub>Sr<sub>x</sub>MnO<sub>3</sub> (x<math>\leq</math>0.5) Studied by Resonant X-ray Scattering at the Mn K Edge.</b> . . . . .	<b>361</b>
G. Subías, J. García, P. Beran, M. C. Sánchez, M. Nevriva, and J. L. García-Muñoz	
<b>Spectroscopic Studies of Electronically-Active Defects in Transition Metal Oxides for Advanced Si Devices</b> . . . . .	<b>364</b>
G. Lucovsky and J. Lüning	

<b>Element Selective X-ray Detected Magnetic Resonance</b> .....	<b>367</b>
J. Goulon, A. Rogalev, F. Wilhelm, N. Jaouen, C. Goulon-Ginet, G. Goujon, J. Ben Youssef, and M. V. Indenbom	
<b>High Pressure X-ray Absorption Spectroscopy on <math>Zn_{1-x}Mn_xO</math> (<math>x=0.25</math> and <math>x=0.05</math>) at the Mn K Edge</b> .....	<b>372</b>
J. P. Itié, A.-M. Flank, P. Lagarde, J. Pellicer-Porres, J. A. Sans, J. F. Sanchez-Royo, A. Segura, and A. Polian	
<b>The Site of In Dopants in Si</b> .....	<b>375</b>
F. d'Acapito, B. Golosio, Y. Shimuzu, S. Scalese, M. Italia, P. Alippi, and S. Grasso	
<b>Mn Occupations in <math>Ga_{1-x}Mn_xN</math> Dilute Magnetic Semiconductors Probed by X-ray Absorption Near-edge Structure Spectroscopy</b> .....	<b>378</b>
S. Wei, W. Yan, Z. Sun, Q. Liu, W. Zhong, X. Zhang, H. Oyanagi, and Z. Wu	
<b>Direct Observation of Nitrogen Location in Molecular Beam Epitaxy Grown Nitrogen-doped ZnO</b> .....	<b>381</b>
P. Fons, H. Tampo, A. V. Kolobov, M. Ohkubo, S. Niki, J. Tominaga, R. Carboni, and S. Friedrich	
<b>Depth-resolved XMCD Application to Fe/Ni/Cu(001) Films</b> .....	<b>384</b>
H. Abe, K. Amemiya, D. Matsumura, T. Ohtsuki, E. Sakai, T. Yokoyama, and T. Ohta	
<b>XAFS Studies and Chemical Shifts of Thallium <math>L_{III}</math> X-ray Absorption Edges in Some of Its Model Compounds and Superconducting Oxides</b> .....	<b>387</b>
A. Agarwal and A. N. Vishnoi	
<b>XAFS Analysis of Local Structure around Ce in <math>Ca_3Sc_2Si_3O_{12}</math>:Ce Phosphor for White LEDs</b> .....	<b>389</b>
T. Akai, M. Shigeiwa, K. Okamoto, Y. Shimomura, N. Kijima, and T. Honma	
<b>Vibrational Properties of Ge Nanocrystals Determined by EXAFS</b> .....	<b>392</b>
L. L. Araujo, P. Kluth, G. de M. Azevedo, and M. C. Ridgway	
<b>XAFS Study of Local Atomic Structure in InAs at Low Pressures</b> .....	<b>395</b>
L. A. Bugaev, Y. V. Latokha, L. A. Avakyan, G. Aquilanti, and S. Pascarelli	
<b>The Pd/Fe Interface in the Epitaxial System Pd/Fe/GaAs(001)- 4 x 6</b> .....	<b>398</b>
P. S. Budnik, R. A. Gordon, and E. D. Crozier	
<b>The Site of Er in Phosphate Glasses Studied by K-Edge EXAFS</b> .....	<b>401</b>
F. d'Acapito, R. Francini, S. Pietrantonio, and D. Barbier	
<b>Local Ordering in Disordered Systems under Extreme Conditions</b> .....	<b>404</b>
A. Di Cicco, E. Principi, M. Minicucci, S. De Panfilis, A. Trapananti, and A. Filipponi	
<b>Thermal Expansion Behaviour of Silver Examined by Extended X-ray Absorption Fine Structure Spectroscopy</b> .....	<b>407</b>
M. Dubiel, A. Chassé, J. Haug, R. Schneider, and H. Kruth	
<b>Cr Atom Alignment in Cr-Delta-Doped GaN</b> .....	<b>410</b>
S. Kimura, S. Emura, H. Ofuchi, Y. Nakata, Y. K. Zhou, S. W. Choi, Y. Yamauchi, S. Hasegawa, and H. Asahi	
<b>An <i>In Situ</i> High Temperature Investigation of Cation Environments in Aluminate and Silicate Glasses and Liquids at the LUCIA Beamline</b> .....	<b>413</b>
D. R. Neuville, L. Cormier, J. Roux, D. de Ligny, A.-M. Flank, G. S. Henderson, and P. Lagarde	
<b>The Silicon Environment in Silica Polymorphs, Aluminosilicate Crystals and Melts: An <i>In Situ</i> High Temperature XAS Study</b> .....	<b>416</b>
L. Courmier, D. R. Neuville, J. Roux, D. de Ligny, G. S. Henderson, A.-M. Flank, and P. Lagarde	
<b>Investigation of Aluminate and <math>Al_2O_3</math> Crystals and Melts at High Temperature Using XANES Spectroscopy</b> .....	<b>419</b>
D. R. Neuville, L. Cormier, J. Roux, G. S. Henderson, D. de Ligny, A.-M. Flank, and P. Lagarde	
<b>EXAFS and XRD Studies with Subpicometer Accuracy: The Case of <math>ReO_3</math></b> .....	<b>422</b>
J. Purans, G. Dalba, P. Fornasini, A. Kuzmin, S. De Panfilis, and F. Rocca	
<b>X-ray Magnetic Circular Dichroism at L Edges of Er in Laves Phase Compounds</b> .....	<b>425</b>
I. Harada, A. Fujiwara, and A. Kotani	
<b>Temperature Dependence of XANES Spectra for <math>ATiO_3</math>, <math>A_2TiO_4</math> and <math>TiO_2</math> Compounds with Structural Phase Transitions</b> .....	<b>428</b>
T. Hashimoto, A. Yoshiasa, M. Okube, H. Okudera, and A. Nakatsuka	
<b>The Influence of the Local Lattice Distortion and Magnetic Ordering in Manganese Oxides on the Mn and O K-XANES</b> .....	<b>431</b>
V. Krayzman, I. Maznickenko, A. Novakovich, and R. Vedrinskii	

<b>Ti K-XANES Analysis of the Cation Distribution in the <math>\text{CaTi}_{1-x}\text{Zr}_x\text{O}_3</math> Solid Solutions</b> .....	434
V. Krayzman, I. Levin, and J. C. Woicik	
<b>EXAFS Study of Semimetal-Semiconductor Transition of Bismuth Clusters</b> .....	437
H. Ikemoto, T. Miyanaga, S. Yoshida, and J. Sogoh	
<b>XAFS Study of the Local Structure of Some Lanthanoid(III) Complexes</b> .....	440
S. Sudoh, T. Miyanaga, and R. Miyamoto	
<b>Fluorescence EXAFS Analysis of SiC:Mn Films Synthesized on SiC Substrates</b> .....	443
H. Ofuchi, W. Wang, F. Takano, and H. Akinaga	
<b>B K-Edge XANES of Superstructural Units in Borate Glasses</b> .....	446
O. Šipr, A. Šimunek, and F. Rocca	
<b>Lattice Defect of Interfacial Layer in Superhard <math>\text{TiN}/\text{Si}_3\text{N}_4</math> Multilayer Films Studied by Fluorescence X-ray Absorption Fine Structure</b> .....	449
Z. Pan, Z. Sun, Z. Xie, J. Xu, I. Kojima, and S. Wei	
<b>Effect of Phosphorus Content on Local Structures of NiP Amorphous Alloys</b> .....	453
J. Song, Z. Wei, Z. Pan, Z. Xie, and S. Wei	
<b>XAFS Studies of Silver Environments in Ion-exchanged Glasses</b> .....	457
X. C. Yang and M. Dubiel	
<b>X-ray Absorption Fine Structure Study for <math>\text{Fe}_{60}\text{Ni}_{40}</math> Alloy</b> .....	460
D.-S. Yang, K. Oh, W. Na, N. Kim, Y.-G. Yoo, S.-G. Min, and S.-C. Yu	
<b>EXAFS and XPS Study of Rutile-Type Difluorides of First-row Transition Metals</b> .....	463
K. I. Murai, Y. Suzuki, T. Moriga, and A. Yoshiasa	
<b>Structural Investigation of Fe-Ni-S and Fe-Ni-Si Melts by High-temperature Fluorescence XAFS Measurements</b> .....	466
M. Manghnani, X. Hong, M. Newville, J. Balogh, and G. Amulele	
<b>Site Determination of Doped Ga Ions in <math>\text{SrTiO}_3:\text{Pr}^{3+}</math> Phosphor for Field Emission Displays by XAFS</b> .....	469
T. Honma and H. Yamamoto	
<b>Magnetic Circular Dichroism of Resonant X-ray Emission Spectroscopy Related to <math>\text{Er}2p \rightarrow 4f</math> Electric Quadrupolar Transition in <math>\text{Er}_3\text{Fe}_5\text{O}_{12}</math></b> .....	472
N. Kawamura, M. Mizumaki, H. Maruyama, and T. Ishikawa	
<b>Selective Study of Atoms in Rough Gold Surfaces by Means of Yoneda-XAFS</b> .....	475
P. Keil, D. Lützenkirchen-Hecht, and R. Frahm	
<b>Observation of Valence State Change in Layered <math>\text{Li}_{1-y}\text{Ni}_{1/3}\text{Mn}_{1/3}\text{Co}_{1/3}\text{O}_2</math></b> .....	478
H. Kobayashi, Y. Arachi, S. Emura, K. Handa, and K. Tatsumi	
<b>EXAFS Study of Disorder in <math>\text{SrTiO}_3</math> Perovskite</b> .....	481
A. Kodre, I. Arčon, J. P. Gomilšek, and B. Zalar	
<b>Identifying Transition Metal Contribution to the Rare-Earth <math>L_2</math>-Edge XMCD Spectra R-T Intermetallics</b> .....	484
M. A. Laguna-Marco, J. Chaboy, C. Piquer, H. Maruyama, N. Ishimatsu, and N. Kawamura	
<b>XAS Studies of Chemical Bonding of Nitrogen and Oxygen Atoms in Ti/Zr/Hf High-K Gate Dielectrics</b> .....	487
H. Seo, S. Lee, B. Ju, G. Lucovsky, and J. Lüning	
<b>Investigation of Room Temperature Oxidation of Cu in Air by Yoneda-XAFS</b> .....	490
P. Keil, D. Lützenkirchen-Hecht, and R. Frahm	
<b>X-ray Absorption Spectroscopy Study of Copper Doped ZnO Thin Films</b> .....	493
Q. Ma, D. B. Buchholz, M. Anderson, L. Agesen, and R. P. H. Chang	
<b>Experimental and Calculated Ti K-Edge XANES Spectra of <math>\text{Pb}_{1-x}\text{La}_x\text{TiO}_3</math> Ferroelectric Ceramic Compounds</b> .....	496
V. R. Mastelaro, P. P. Neves, A. Michalowicz, and J. A. Eiras	
<b>Local Structure around In Atoms in <math>\text{In}_x\text{Ga}_{1-x}</math> N Multi-Quantum-Wells Studied by XAFS</b> .....	499
S. Sasaki, T. Miyanaga, T. Azuhata, T. Uruga, H. Tanida, S. F. Chichibu, and T. Sota	
<b>Measurements and Theoretical Calculations of Magnetic XAFS for Ni-Mn Alloys in Ordered and Disordered States</b> .....	502
T. Miyanaga, T. Ogasawara, T. Okazaki, Y. Sakisaka, K. Okamoto, S. Nagamatsu, and T. Fujikawa	
<b>Spin Reorientation Transition in Ultrathin Co Films on Ru(0001) Induced by Ru Capping</b> .....	505
J. Miyawaki, D. Matsumura, H. Abe, T. Otsuki, E. Sakai, K. Amemiya, and T. Ohta	
<b>Li K-Edge XANES Spectra of Lithium Niobate and Lithium Tantalite</b> .....	508
H. Mizota, Y. Ito, T. Tochio, K. Handa, S. Takekawa, and K. Kitamura	

<b>Soft X-ray Absorption Spectroscopy of High-abrasion-furnace Carbon Black</b> .....	<b>511</b>
Y. Muramatsu, R. Harada, and E. M. Gullikson	
<b>Multiple Scattering Approach to Polarization Dependence of F K-Edge XANES Spectra for Highly Oriented Polytetrafluoroethylene (PTFE) Thin Film</b> .....	<b>514</b>
S. Nagamatsu, M. Ono, S. Kera, K. K. Okudaira, T. Fujikawa, and N. Ueno	
<b>Fluorescence XAFS Study on Local Structure around Cr Atoms Doped in ZnTe</b> .....	<b>517</b>
H. Ofuchi, N. Ozaki, N. Nishizawa, H. Kinjyo, S. Kuroda, and K. Takita	
<b>Analysis of the Local Structure around Eu and Mn Ions in Alkaline-Earth Silicate Phosphors for White Light Illumination</b> .....	<b>520</b>
K. Okamoto, M. Yoshino, M. Shigeiwa, M. Mikami, T. Akai, N. Kijima, T. Honma, and M. Nomura	
<b>Direct Evidence for Trivalent Titanium in Artificially Irradiated (Electrons) Oxide Glasses</b> .....	<b>523</b>
N. Ollier, F. Farges, B. Boizot, P. Lombard, A.-M. Flank, and P. Lagarde	
<b>X-ray Induced Magnetic Phase Transition in CoW Cyanide Probed by XMCD</b> .....	<b>526</b>
H. Osawa, N. Kawamura, T. Matsuda, Y. Arimoto, H. Tokoro, K. Hashimoto, and S. I. Ohkoshi	
<b>Al Thermal Diffusion in <math>\alpha</math>-Si<sub>1-x</sub>C<sub>x</sub>:H Thin Film Studied by XAFS</b> .....	<b>529</b>
R. J. Prado, M. C. A. Fantini, M. N. P. Carreño, I. Pereyra, and A.-M. Flank	
<b>Metastable Bi under Extreme Conditions Investigated by Combined XAS and XRD</b> .....	<b>532</b>
E. Principi, M. Minicucci, A. Di Cicco, A. Trapananti, S. De Panfilis, and R. Poloni	
<b>High-throughput Synthesis and Characterization of BiMoVOX Materials</b> .....	<b>535</b>
S. Russu, M. Tromp, N. Tsapatsaris, A. M. Beesley, S. L. M. Schroeder, M. T. Weller, and J. Evans	
<b>X-ray Absorption Near-edge Structure (XANES) of Calcium L<sub>3,2</sub> Edges of Various Calcium Compounds and X-ray Excited Optical Luminescence (XEOL) Studies of Luminescent Calcium Compounds</b> .....	<b>538</b>
J. Y. P. Ko, X.-T. Zhou, F. Heigl, T. Regier, R. I. R. Blyth, and T.-K. Sham	
<b>XMCD of Oxygen Adsorbates on Fe, Co, and Ni Monolayers</b> .....	<b>541</b>
C. Sorg, N. Ponpandian, J. Luo, R. Q. Wu, M. Bernien, K. Baberschke, and H. Wende	
<b>Local Structural Distortions Inducing Resonant Forbidden Reflections in LaMnO<sub>3</sub></b> .....	<b>544</b>
G. Subías, J. Herrero-Martín, J. García, J. Blasco, M. C. Sánchez, C. Mazzoli, S. Di Matteo, K. Hatada, and C. R. Natoli	
<b>Local Lattice Distortion of Ge Impurity in Si (001): Multiple-Scattering EXAFS Study</b> .....	<b>547</b>
Z. Sun, W. Yan, H. Oyanagi, Z. Pan, and S. Wei	
<b>EXAFS Analysis of the Local Structure of Cd<sub>(1-x)</sub>M<sub>x</sub>Te (M=Cr, Fe, Ni)</b> .....	<b>550</b>
N. E. Sung, H.-Y. Park, and M.-S. Jang	
<b>XAFS and XRD Study of the Atomic Displacements in Aurivillius Phase Ferroelectric Bi<sub>2.25</sub>Ca<sub>0.5</sub>Na<sub>0.25</sub>Nb<sub>2</sub>O<sub>9</sub></b> .....	<b>553</b>
V. G. Vlasenko, A. T. Shuvaev, I. V. Pirog, D. Drannikov, and I. A. Zarubin	
<b>In Situ XANES Study of CuO/TiO<sub>2</sub> Thin Films During Photodegradation of Methylene Blue</b> .....	<b>556</b>
T. L. Hsiung, H. P. Wang, and Y.-L. Wei	
<b>Ge Migration Effect of Si/Ge<sub>n</sub>/Si(100) Heterostructure Films Probed by Grazing Incidence Fluorescence X-ray Absorption Fine Structure</b> .....	<b>559</b>
Z. Pan, H. Oyanagi, Z. Sun, Z. Xie, J. Fan, and S. Wei	
<b>Atomic-scale Structure of Al<sub>2</sub>O<sub>3</sub>-ZrO<sub>2</sub> Mixed Oxides Prepared by Laser Ablation</b> .....	<b>563</b>
X. Yang, M. Dubiel, H. Hofmeister, and W. Riehemann	
<b>EXAFS Analysis of the Local Structure of Ge<sub>x</sub>Si<sub>1-x</sub> Thin Film Alloys</b> .....	<b>566</b>
N. Sung, Y.-G. Yoo, and D.-S. Yang	
<b>Pressure Dependence of Anharmonic Effective Pair Potentials in Rock Salt Type AgI</b> .....	<b>569</b>
A. Yoshiasa, H. Fukui, H. Arima, M. Okube, Y. Katayama, K.-I. Murai, M. Sugahara, and O. Ohtaka	
<b>Measurement of Soft X-ray Excited Optical Luminescence of a Silica Glass</b> .....	<b>572</b>
T. Yoshida, S. Muto, and T. Tanabe	

## CATALYSIS

<b>Time-resolved and Operando XAS Studies on Heterogeneous Catalysts—From the Gas Phase Towards Reactions in Supercritical Fluids</b> .....	<b>577</b>
J.-D. Grunwaldt and A. Baiker	
<b>Electronic and Geometric Structure of Small Gold Metal Particles: Particles Size Effects and the Relationship to Catalytic Activity</b> .....	<b>582</b>
J. A. van Bokhoven and J. T. Miller	

<b>Following the Formation of Active Co(III) Sites in Cobalt Substituted Aluminophosphates Catalysts by <i>In-Situ</i> Combined UV-VIS/XAFS/XRD Technique</b> .....	<b>585</b>
G. Sankar, S. Fiddy, A. M. Beale, I. Harvey, S. Hayama, and G. Bushnell-Wye	
<b>State-sensitive Monitoring of Active and Promoter Sites. Applications to Au/Titania and Pt-Sn/Silica Catalysts by XAFS Combined with X-ray Fluorescence Spectrometry</b> .....	<b>588</b>
Y. Izumi, D. Masih, J.-P. Candy, H. Yoshitake, Y. Terada, H. Tanida, and T. Uruga	
<b>Size and Shape of Rhenium Nanoparticles</b> .....	<b>591</b>
N. Yang, G. E. Mickelson, N. Greenlay, S. D. Kelly, F. D. Vila, J. Kas, J. J. Rehr, and S. R. Bare	
<b>Real-time Observation of Platinum Redispersion on Ceria-Based Oxide by <i>In Situ</i> Turbo-XAS in Fluorescence Mode</b> .....	<b>594</b>
Y. Nagai, N. Takagi, Y. Ikeda, K. Dohmae, T. Tanabe, G. Guilera, S. Pascarelli, M. Newton, H. Shinjoh, and S. Matsumoto	
<b>High Throughput <i>In Situ</i> XAFS Screening of Catalysts</b> .....	<b>597</b>
N. Tsapatsaris, A. M. Beesley, N. Weiher, H. Tatton, A. J. Dent, F. J. W. Mosselmans, M. Tromp, S. Russu, J. Evans, I. Harvey, S. Hayama, and S. L. M. Schroeder	
<b><i>In Situ</i> XAS Studies on the Structure of the Active Site of Supported Gold Catalysts</b> .....	<b>600</b>
N. Weiher, A. M. Beesley, N. Tsapatsaris, C. Louis, L. Delannoy, J. A. van Bokhoven, and S. L. M. Schroeder	
<b><i>In Situ</i> Structure-function Studies of Oxide Supported Rhodium Catalysis by Combined Energy Dispersive XAFS and DRIFTS Spectroscopies</b> .....	<b>603</b>
J. Evans, A. J. Dent, S. Diaz-Moreno, S. G. Fiddy, B. Jyoti, M. A. Newton, and M. Tromp	
<b>Dispersive XAS on a High Brilliance Source: Highlights and Future Opportunities</b> .....	<b>608</b>
S. Pascarelli, G. Aquilanti, L. Dubrovinsky, G. Guilera, O. Mathon, M. Muñoz, M. A. Newton, M. Pasquale, and A. Trapananti	
<b>Structure of Ti in TiCl<sub>3</sub> Doped NaAlH<sub>4</sub></b> .....	<b>613</b>
C. P. Baldé, H. A. Stil, A. M. J. van der Eerden, K. P. de Jong, and J. H. Bitter	
<b><i>In Situ</i> EXAFS Studies on Ni<sub>2</sub>P Hydrodesulfurization Catalysts in the Presence of High Pressure and High Temperature Oil</b> .....	<b>616</b>
T. Kawai, K. K. Bando, Y.-K. Lee, S. T. Oyama, W.-J. Chun, and K. Asakura	
<b>ED-XAS Data Reveal <i>In-Situ</i> Time-resolved Adsorbate Coverage on Supported Molybdenum Oxide Catalysts during Propane Dehydrogenation</b> .....	<b>619</b>
D. Ramaker, D. Gatewood, A. M. Beale, and B. M. Weckhuysen	
<b>Design and Operation of an <i>In Situ</i> High Pressure Reaction Cell for X-ray Absorption Spectroscopy</b> .....	<b>622</b>
S. R. Bare, N. Yang, S. D. Kelly, G. E. Mickelson, and F. S. Modica	
<b>Theoretical XANES Study of the Activated Nickel (t-Amylisocyanide) Molecule</b> .....	<b>625</b>
J. L. Glover, C. T. Chantler, A. V. Soldatov, G. Smolentsev, and M. C. Feiters	
<b>Structural Characterization of AgGaS<sub>2</sub>-type Photocatalysts for Hydrogen Production from Water under Visible Light</b> .....	<b>628</b>
S. H. Choi, J. S. Jang, N. Shin, and J. S. Lee	
<b>Characterization of Binary Ag-Cu Ion Mixtures in Zeolites: Their Reduction Products and Stability to Air Oxidation</b> .....	<b>631</b>
S. Fiddy, V. Petranovskii, S. Ogden, and I. R. Iznaga	
<b>New Highly Mixed Phases in Ball-Milled Cu/ZnO Catalysts as Established by EXAFS and XANES</b> .....	<b>636</b>
D. Grandjean, H. L. Castricum, J. C. van den Heuvel, and B. M. Weckhuysen	
<b><i>In-Situ</i> XAFS Characterization for Nitriding Process of Silica Supported Nb Catalysts under N<sub>2</sub>-H<sub>2</sub> Gas</b> .....	<b>639</b>
N. Ichikuni, H. Matsumoto, H. Haneishi, K. K. Bando, and S. Shimazu	
<b>Spatial Configurations of Ti- and Ni- Species Catalyzing Complex Metal Hydrides: X-ray Absorption Studies and First-principles DFT and MD Calculations</b> .....	<b>642</b>
A. Y. Ignatov, J. Graetz, S. Chaudhuri, T. T. Salguero, J. J. Vajo, M. S. Meyer, F. E. Pinkerton, and T. A. Tyson	
<b>XAFS Analysis of Pt and Pt-Ru Catalysts for PEFCs by <i>In-Situ</i> Measurements under Operating Conditions in the Fluorescence Mode</b> .....	<b>645</b>
H. Kageyama, T. Ioroi, T. Kojima, H. Senoh, N. Takeichi, K. Nomura, and K. Tanimoto	

<b>The Chemical Composition and Structure of Supported Sulfated Zirconia with Regulated Size Nanoparticles</b> .....	<b>648</b>
V. V. Kanazhevskiy, V. P. Shmachkova, N. S. Kotsarenko, D. I. Kochubey, and J. C. Vedrine	
<b>High Energy Resolution Fluorescence Detection X-ray Absorption Spectroscopy: Detection of Adsorption Sites in Supported Metal Catalysts</b> .....	<b>651</b>
M. Tromp, J. A. van Bokhoven, O. V. Safonova, F. M. F. de Groot, J. Evans, and P. Glatzel	
<b>Application of <i>In-Situ</i> High Energy-resolution Fluorescence Detection and Time-resolved X-ray Spectroscopy: Catalytic Activation of Oxygen over Supported Gold Catalysts</b> .....	<b>654</b>
J. A. van Bokhoven, M. Tromp, P. Glatzel, and O. Safonova	
<b>Effect of Silica Surface Area on Molecular Structures of Lead in Thermally Treated Mixtures of Lead Acetate and Silica Oxide</b> .....	<b>657</b>
Y.-L. Wei, K.-W. Cheng, N. Cheng, and H. P. Wang	
<b>XAFS Study on Nano-sized Pd Metal Catalyst Deposited on Ti-containing Zeolite by a Photo-assisted Deposition (PAD) Method</b> .....	<b>660</b>
H. Yamashita, Y. Miura, M. Tomonari, Y. Masui, and K. Mori	
<b><i>In Situ</i> XAS of Ni-W Hydrocracking Catalysts</b> .....	<b>663</b>
N. Yang, G. E. Mickelson, N. Greenlay, S. D. Kelly, and S. R. Bare	
<b>Unraveling the Structure of Mn-promoted Co/TiO<sub>2</sub> Fischer-Tropsch Catalysts by <i>In Situ</i> X-ray Absorption Spectroscopy</b> .....	<b>666</b>
D. Grandjean, F. Morales, A. Mens, F. M. F. de Groot, and B. M. Weckhuysen	
<b><i>In Situ</i> Monitoring of Ni-based Catalysts during the Synthesis of Propylene Carbonate</b> .....	<b>669</b>
M. Ramin, S. Reimann, J.-D. Grunwaldt, and A. Baiker	
<b>XAFS Study of the Photo-active Site of Mo/MCM-41</b> .....	<b>672</b>
D. Miyamoto, N. Ichikuni, and S. Shimazu	
<b>Time-resolved DXAFS Study of Adsorption and Release of Hydrogen on Pt/MCM- 41</b> .....	<b>675</b>
A. Suzuki, Y. Inada, K. Asakura, and M. Nomura	
<b>XAFS Study on Deterioration of Cathode Materials for Lithium-ion Batteries</b> .....	<b>678</b>
T. Nonaka, C. Okuda, Y. Kondo, Y. Seno, and Y. Ukyo	
<b>XAS Study at Mo and Co K-Edges of the Sulfidation of a CoMo/Al<sub>2</sub>O<sub>3</sub> Hydrotreating Catalyst</b> .....	<b>681</b>
C. Pichon, A. D. Gandubert, C. Legens, and D. Guillaume	
<b>Advanced XAS Analysis for Investigating Fuel Cell Electrocatalysts</b> .....	<b>684</b>
A. Witkowska, E. Principi, A. Di Cicco, and R. Marassi	
<b>X-ray Excited Optical Luminescence from Ru(bipy)<sub>3</sub><sup>2+</sup> and Ru(phen)<sub>3</sub><sup>2+</sup> in the Energy and Time Domains</b> .....	<b>687</b>
S. Lam, F. Heigl, P.-S. G. Kim, T. K. Sham, R. A. Gordon, D. Brewé, T. Regier, I. Coulthard, and R. I. R. Blyth	
<b>Energy-dispersive XAFS Study on Reduction Behavior of Pt Supported on TiO<sub>2</sub> and Al<sub>2</sub>O<sub>3</sub></b> .....	<b>690</b>
T. Shishido, F. Amano, T. Sone, S. Yamazoe, K. Kato, K. Teramura, and T. Tanaka	
<b>An <i>In-Situ</i> XAS Study of the Structural Changes in a CuO-CeO<sub>2</sub>/Al<sub>2</sub>O<sub>3</sub> Catalyst during Total Oxidation of Propane</b> .....	<b>693</b>
G. Silversmit, M. Olea, H. Poelman, V. Balcaen, P. Heynderickx, D. Poelman, R. De Gryse, and G. B. Marin	
<b>XAFS Study of Active Tungsten Species on WO<sub>3</sub>/TiO<sub>2</sub> as a Catalyst for Photo-SCR</b> .....	<b>696</b>
S. Yamazoe, Y. Masutani, T. Shishido, and T. Tanaka	
<b>Cr K-Edge XANES Spectroscopy: Ligand and Oxidation State Dependence—What is Oxidation State?</b> .....	<b>699</b>
M. Tromp, J. Moulin, G. Reid, and J. Evans	
<b>Structure of Catalytically Active Sites in Supported Metal Catalysts</b> .....	<b>702</b>
J. A. van Bokhoven, E. Bus, and D. E. Ramaker	
<b>Speciation of Raney Copper Oxide during High-temperature Desulfurization</b> .....	<b>705</b>
T. C. Wang, H. P. Wang, C. Y. Chen, H.-L. Huang, and Y.-L. Wei	
<b>XAFS Study on TiO<sub>2</sub> Photocatalyst Loaded on Zeolite Synthesized from Steel Slag</b> .....	<b>708</b>
Y. Kuwahara, T. Ohmichi, K. Mori, I. Katayama, and H. Yamashita	
<b>Pd-Pt Catalysts on Fluorinated Alumina Support Studied by X-ray Absorption Fine Structure</b> .....	<b>711</b>
W. Yan, Z. Li, Z. Wei, and S. Wei	
<b>XAFS Study of HY Zeolite Supported Pt Nanoparticle Catalysts Prepared with Different Methods</b> .....	<b>714</b>
Z. Li, W. Yan, and S. Wei	

<b>Oxygen K-Edge Emission and Absorption Spectroscopy of Iron Oxyhydroxide Nanoparticles</b> . . . . .	<b>721</b>
B. Gilbert, C. S. Kim, C.-L. Dong, J. Guo, P. S. Nico, and D. K. Shuh	
<b>Study of Interactions between Microbes and Minerals by Scanning Transmission X-ray Microscopy (STXM)</b> . . . . .	<b>726</b>
K. Benzerara, T. Tyliszczak, and G. E. Brown, Jr.	
<b>Vibrational Properties of Au and Cu Nanocrystals Formed by Ion Implantation</b> . . . . .	<b>731</b>
P. Kluth, B. Johannessen, L. L. Araujo, and M. C. Ridgway	
<b>Optical XAFS of ZnO Nanowires at the Zn K-Edge and Related Phenomena</b> . . . . .	<b>734</b>
F. Heigl, X. H. J. Sun, S. Lam, T.-K. Sham, R. Gordon, D. Brewre, R. Rosenberg, G. Shenoy, M. Yablonskikh, J. MacNaughton, and A. Moewes	
<b>EXAFS Characterization of Dendrimer-Derived Pt/<math>\gamma</math>-Al<sub>2</sub>O<sub>3</sub></b> . . . . .	<b>737</b>
A. Siani, O. S. Alexeev, C. T. Williams, H. J. Ploehn, and M. D. Amiridis	
<b>Alternation of the Pd Lattice in Nano-sized-Pd/ZrO<sub>2</sub> Composite during Hydrogen Absorption</b> . . . . .	<b>740</b>
Y. Arachi, S. Emura, A. Omura, M. Nunogaki, T. Asai, S. Yamaura, A. Inoue, and Y. Arata	
<b><i>In Situ</i> EXAFS and TEM Investigations of Ag Nanoparticles in Glass</b> . . . . .	<b>743</b>
R. Schneider, M. Dubiel, J. Haug, and H. Hofmeister	
<b>Geometrical Characteristics of Regular Polyhedra: Application to EXAFS Studies of Nanoclusters</b> . . . . .	<b>746</b>
D. Glasner and A. I. Frenkel	
<b>Geometry and Charge State of Mixed-Ligand Au<sub>13</sub> Nanoclusters</b> . . . . .	<b>749</b>
A. I. Frenkel, L. D. Menard, P. Northrup, J. A. Rodriguez, F. Zypman, D. Glasner, S.-P. Gao, H. Xu, J. C. Yang, and R. G. Nuzzo	
<b>EXAFS Studies of Palladium Nanoparticles: Size Control and Hydrogenation</b> . . . . .	<b>752</b>
T. Harris, L. Soussan, R. Isseroff, Y. Sun, M. H. Rafailovich, and A. I. Frenkel	
<b>Micromagnetic Aspects of Magnetoreception of Homing Pigeons Based on Iron Minerals</b> . . . . .	<b>755</b>
B. Stahl, G. Fleissner, G. Fleissner, and E. Holub-Krappe	
<b>Effect of Precursor on the Electronic and Geometric Properties of Cobalt Nanoparticles Investigated by Co-K XANES and EXAFS</b> . . . . .	<b>758</b>
V. Palshin, R. M. de Silva, J. Hormes, and C. S. S. R. Kumar	
<b>X-ray Absorption Microspectroscopy with Electrostatic Force Microscopy and Its Application to Chemical States Mapping</b> . . . . .	<b>761</b>
M. Ishii, N. Rigopoulos, N. R. J. Poolton, and B. Hamilton	
<b>An X-ray Excited Optical Luminescence (XEOL) Analysis of Mn<sup>2+</sup> Doped ZnS Nanostructures</b> . . . . .	<b>764</b>
M. Murphy, X.-T. Zhou, F. Heigl, T. Regier, and T.-K. Sham	
<b>Support Effects on Electronic Behaviors of Gold Nanoparticles Studied by X-ray Absorption Fine Structure</b> . . . . .	<b>767</b>
Z.-R. Li, W. Yan, and S. Wei	
<b><i>In-Situ</i> XAFS Investigation of the Crystallization Mechanism of Ni-B Nano-Amorphous Alloy</b> . . . . .	<b>771</b>
Z. Wei, Z. Jiang, J. Ye, W. Zhong, J. Song, and S. Wei	
<b>XAFS Study on Ag<sub>2</sub>S Semiconductor Clusters Designed in Nanopores and Their Photoluminescence Properties</b> . . . . .	<b>774</b>
S. Yuan, M. Tomonari, D. Matsuo, K. Mori, T. Ohmichi, I. Katayama, and H. Yamashita	
<b>Origin of the Luminescence from SnO<sub>2</sub> Nanoribbons</b> . . . . .	<b>777</b>
X. T. Zhou, F. Heigl, M. W. Murphy, T. Regier, I. Coulthard, R. I. R. Blyth, and T. K. Sham	
<b>XAFS Studies of Fe Doped PbTiO<sub>3</sub> Nanoparticles</b> . . . . .	<b>780</b>
T. Shibata, S. Chattopadhyay, B. Lin, and V. R. Palkar	
<b>Mn K-edge XMCD Study of the Mixed-valence State of Mn-based Molecular Nanomagnets</b> . . . . .	<b>783</b>
G. Subías, J. García, and M. C. Sánchez	
<b>Ni K-edge XANES Analyses of Residual Ni Catalyst in Carbon Nanofiber Using Full Multiple Scattering Theory</b> . . . . .	<b>786</b>
M. Ushiro, K. Asakura, K. Ohminami, S. I. Nagamatsu, and T. Fujikawa	
<b>Abstraction of Nano Copper in a Room-temperature Ionic Liquid</b> . . . . .	<b>789</b>
C. Y. Peng, H. P. Wang, C. H. Huang, and Y.-L. Wei	
<b>Structure Evolution of CdSe Nanocrystals during Ripening Process Studied by XAFS</b> . . . . .	<b>792</b>
X. Zhang, F. Wei, W. Yan, and S. Wei	



<b>Local Structures of Mechanically Alloyed Al<sub>70</sub>Cu<sub>20</sub>Fe<sub>10</sub> Nanocomposites Studied by XRD and XAFS</b> .....	795
S. Yin, L. Qian, B. He, S. Zou, Q. Bian, and S. Wei	
<b>XAFS Study on Nano-sized Metal Catalyst Prepared by a Photo-assisted Deposition Using Ti-containing Mesoporous Silica Thin Film Photocatalyst</b> .....	799
M. Shimada, S. Nishio, T. Shimuzi, K. Mori, T. Ohmichi, I. Katayama, and H. Yamashita	
<b>Formation Mechanism of Ge Nanocrystals Embedded in SiO<sub>2</sub> Studied by Fluorescence X-ray Absorption Fine Structure</b> .....	802
W. Yan, Z. Li, Z. Sun, A. V. Kolobov, and S. Wei	
<b>XAFS and XEOL Studies of CdSe Nanostructures</b> .....	806
J. G. Zhou, X. H. Sun, X. T. Zhou, M. Murphy, F. Heigl, Z. F. Ding, and T. K. Sham	
<b>EXAFS Studies of Nanocrystals of Zn<sub>1-x</sub>Mn<sub>x</sub>O: A Dilute Magnetic Semiconductor Oxide System</b> .....	809
S. Chattopadhyay, S. D. Kelly, T. Shibata, R. Viswanatha, M. Balasubramanian, S. Stoupin, C. U. Segre, and D. D. Sarma	

## CHEMICAL SYSTEMS

<b><i>Ab Initio</i> Calculations for Inner-shell Ionized and Excited States of Molecular Pyridine Clusters</b> .....	815
I. Bradeanu and N. Kosugi	
<b>Observing the Influence of X-rays on Aqueous Copper Solutions by <i>In Situ</i> Combined Video/XAFS/UV-Vis Spectroscopy</b> .....	818
J. G. Mesu, A. M. Beale, F. M. F. de Groot, and B. M. Weckhuysen	
<b>EXAFS Studies of Some Copper(II) Mixed-ligand Complexes</b> .....	821
S. K. Joshi, R. K. Katare, and B. D. Shrivastava	
<b>Characterization of Sulfur Compounds in Coffee Beans by Sulfur K-XANES Spectroscopy</b> .....	824
H. Lichtenberg, A. Prange, H. Modrow, and J. Hormes	
<b>Structure-property Relationships in Solid AlF<sub>3</sub> Lewis Acids</b> .....	827
N. Weiher, A. Makarowicz, A. M. Beesley, E. Kemnitz, and S. L. M. Schroeder	

## NOVEL METHODS

<b>Selective XAFS Studies of Functional Materials by Resonant Inelastic X-ray Scattering</b> .....	833
H. Hayashi	
<b>An Introduction to Differential EXAFS</b> .....	838
M. P. Ruffoni, R. F. Pettifer, S. Pascarelli, A. Trapananti, and O. Mathon	
<b>Temperature Scanning Techniques with Tunable X-ray Photons</b> .....	841
A. Filipponi, S. De Panfilis, and A. Di Cicco	
<b>Molecular Structural Dynamics of Photoactive Transition Metal Complexes in Solar Energy Conversion Studied by Ultrafast Optical Spectroscopy and LITR-XAS</b> .....	844
L. X. Chen, G. B. Shaw, E. C. Wasinger, X. Zhang, K. Attenkofer, and G. Jennings	
<b>Time-resolved X-ray Absorption Spectroscopy Data for the Study of Chemical Reaction Intermediate States</b> .....	849
S. Diaz-Moreno, D. T. Bowron, and J. Evans	
<b>Micro-soft X-ray Spectroscopy with the LUCIA Beamline</b> .....	852
P. Lagarde, A.-M. Flank, D. Vantelon, and M. Janousch	
<b>High-throughput Structure/Function Screening of Materials and Catalysts with Multiple Spectroscopic Techniques</b> .....	858
M. Tromp, S. Russu, A. J. Dent, J. F. W. Mosselmans, I. Harvey, S. Hayama, A. E. Russell, S. Guerin, B. E. Hayden, J.-P. Suchsland, K. Meacham, M. SurrIDGE, J. G. Frey, N. Tsapatsaris, A. M. Beesley, S. L. M. Schroeder, M. A. Newton, S. Fiddy, O. V. Safonova, P. Glatzel, N. Binsted, and J. Evans	
<b>Spin-sensitive and Angular Dependent Detection of Resonant Excitations at the K Absorption Pre-edge of <math>\alpha</math>-Fe<sub>2</sub>O<sub>3</sub></b> .....	861
P. Glatzel, A. Mirone, S. G. Eeckhout, M. Sikora, and G. Giuli	

<b>Time Resolved Studies of ZnO (Eu) Nanostructure Luminescence Using Short Synchrotron Radiation Pulses</b> . . . . .	<b>864</b>
F. Heigl, A. Jürgensen, X.-T. Zhou, M. Murphy, J. Y. P. Ko, S. Lam, T. K. Sham, T. Regier, R. I. R. Blyth, I. Coulthard, L. Zuin, Y.-F. Hu, L. Armelao, R. A. Gordon, and D. Brewé	

## INSTRUMENTATION

<b>Simultaneous Detection of X-ray Fluorescence and Conversion Electrons for Depth Selective XAFS Analysis</b> . . . . .	<b>869</b>
S. Hayakawa, Y. Makiyama, T. Esumi, S. Qiao, A. Morikawa, S. Tohno, H. Namatame, and T. Hirokawa	
<b>Proxima 1, a New Beamline on the Third Generation SR Source SOLEIL Combining PX and Single-crystal BioXAS</b> . . . . .	<b>872</b>
I. Ascone, E. Girard, P. Gourhant, P. Legrand, O. Roudenko, L. Roussier, and A. W. Thompson	
<b>The INE-Beamline for Actinide Research at ANKA</b> . . . . .	<b>875</b>
B. Brendebach, M. A. Denecke, J. Rothe, K. Dardenne, and J. Römer	
<b>Advantages of an Automated Chemical Processor for XAFS Analysis of Novel Materials</b> . . . . .	<b>878</b>
S. Calvin and E. E. Carpenter	
<b>New 36-element Pixel Array Detector at the ANBF—Choosing the Right Detector for Your Beamline</b> . . . . .	<b>881</b>
G. Foran, J. Hester, R. Garrett, P. Dressler, C. Fonne, J.-O. Beau, and M.-O. Lampert	
<b>Status of the X-ray Absorption Spectroscopy (XAS) Beamline at the Australian Synchrotron</b> . . . . .	<b>884</b>
C. Glover, J. McKinlay, M. Clift, B. Barg, J. Boldeman, M. Ridgway, G. Foran, R. Garrett, P. Lay, and A. Broadbent	
<b>Characteristics of the MBE1 End-Station at PNC/XOR</b> . . . . .	<b>887</b>
R. Gordon, E. D. Crozier, D.-T. Jiang, J. Shoults, B. Barg, and P. S. Budnik	
<b>An XAFS Beamline at the SAGA Light Source</b> . . . . .	<b>890</b>
T. Okajima, K. Hara, M. Tabata, H. Setoyama, D. Yoshimura, and Y. Chikaura	
<b>XAFS at the Canadian Light Source</b> . . . . .	<b>893</b>
D. T. Jiang, N. Chen, L. Zhang, K. Malgorzata, G. Wright, R. Igarashi, D. Beauregard, M. Kirkham, and M. McKibben	
<b>A New XAFS Beamline NW10A at the Photon Factory</b> . . . . .	<b>896</b>
M. Nomura, Y. Koike, M. Sato, A. Koyama, Y. Inada, and K. Asakura	
<b>Fluorescence XAS Using Ge PAD: Application to High-temperature Superconducting Thin Film Single Crystals</b> . . . . .	<b>899</b>
H. Oyanagi, A. Tsukada, M. Naito, N. L. Saini, and C. Zhang	
<b>Performance and Improved Design of the Log Spiral of Revolution Monochromator</b> . . . . .	<b>902</b>
D. Pease, A. I. Frenkel, P. Shanthakumar, T. Huang, M. Balasubramanian, J. I. Budnick, D. Brewé, N. Abitbol, and O. Odong	
<b>New XAFS Facility for In-Situ Measurements at Beamline C at HASYLAB</b> . . . . .	<b>905</b>
K. Rickers, W. Drube, H. Schulte-Schrepping, E. Welter, U. Brüggemann, M. Herrmann, J. Heuer, and H. Schulz-Ritter	
<b>Novel Preparation Methods for the Fabrication of Thin-film EXAFS Samples</b> . . . . .	<b>908</b>
M. C. Ridgway, C. J. Glover, P. Kluth, B. Johannessen, and G. J. Foran	
<b>The LERIX User Facility</b> . . . . .	<b>911</b>
G. T. Seidler, T. T. Fister, J. O. Cross, and K. P. Nagle	
<b>Quick XAFS System Using Quasimonochromatic Undulator Radiation at SPring-8</b> . . . . .	<b>914</b>
T. Uruga, H. Tanida, K. Inoue, H. Yamazaki, and T. Irie	
<b>Development of a New Silicon Drift Detector Module</b> . . . . .	<b>917</b>
E. Welter and K. Hansen	
<b>An Ion Chamber Dedicated to Carbon NEXAFS: Removal of High-order X-rays and Reliable Flux Measurement</b> . . . . .	<b>920</b>
L.-J. Fan, Y.-W. Yang, and K. Lee	
<b>Performance of Multilayer Array Analyzer Detector in the Intermediate Energy Region (1 KeV to 3 KeV)</b> . . . . .	<b>923</b>
K. Zhang, G. Rosenbaum, Q. Liu, and D. Fischer	
<b>Author Index</b> . . . . .	<b>927</b>

## Preface

At the XAFS11 Conference in Aso, in 2000, Stanford Synchrotron Radiation Laboratory (SSRL) was selected as host and organizer for the 13<sup>th</sup> International Conference on X-ray Absorption Fine Structure, or XAFS13. With the highly successful 2003 XAFS12 conference in Malmö, Sweden in mind, we initiated the XAFS13 preparations in 2005. The planning and organizational process culminated in meeting colleagues and friends at the Frances C. Arrillaga Alumni Center on Stanford University main campus during the warm and sunny week of July 9-14, 2006, to listen to talks, view posters - and to engage in personal scientific interactions that is one of the most important outcomes of international meetings. This book represents the Proceedings of this conference. It is introduced by a Conference overview of the science and program by Prof. Gordon Brown, Jr. This is followed by the first section of papers, devoted to the opening symposium in the honor of the late Dale Sayers. Thereafter are 10 broadly defined scientific sections of papers that focus on Plenary Talks, Theory & Modeling, Environmental & Earth Science, Biological & Medical, Materials & Magnetism, Catalysis, Nano, Chemical Science, Novel Methods, and Instrumentation, respectively. In all, these Proceedings represent about 60% of the conference presentations. We hope that these Proceedings will be of high value to the growing XAFS community. We believe that they serve as an indicator of present trends and developments, as well as an illustration of the continued extensive impact of XAFS tools and synchrotron sources in many areas of science.

We gratefully acknowledge the support from our main conference sponsors, Stanford University, Stanford Linear Accelerator Center, Stanford Synchrotron Radiation Laboratory, and at a large number of our sister light sources around the world; the program guidance from the International Advisory Committee; the work by the local Program Committee chaired by Prof. Ingolf Lindau; the interactions with the IXS Executive Committee; and the outstanding support from our SSRL administrative staff, named in the Conference overview. We also acknowledge the support of SLAC's InfoMedia Solution's team members Terry Anderson for logo and graphic designs, and Sharon West and Yasuko Weyhrauch for editing and production for this Proceedings and pre-conference publications. Finally – we thank all the participants and authors for an exciting meeting, for their contributions to these proceedings, and for their cooperation during the peer-review and editorial processes.

Stanford, November 2006  
Britt Hedman  
Piero Pianetta

# Conference Committees

## International Advisory Committee

Dimitri Arvanitis, Sweden  
Klaus Baberschke, Germany  
Majed Chergui, Switzerland  
Jinho Choy, Korea  
Andrea Di Cicco, Italy  
Francois Farges, France  
Ronald Frahm, Germany  
Graham N George, Canada  
Neville Greaves, United Kingdom  
Chi-Chang Kao, USA  
Olof Karis, Sweden  
Janos Kirz, USA  
Diek C Koningsberger, Netherlands  
Peter A Lay, Australia

Alain Manceau, France  
Alfons Molenbroek, Denmark  
Toshiaki Ohta, Japan  
Hiroyuki Oyanagi, Japan  
Andrej Pavlychev, Russia  
James E Penner-Hahn, USA  
Denis Raoux, France  
John J Rehr, USA  
Dipankar Das Sarma, India  
George Sawatsky, Canada  
Tsun-Kong Sham, Canada  
Steve Sutton, USA  
Helio Tolentino, Brazil  
Ziyu Wu, China

## Program Committee

John R Bargar, SSRL  
Uwe Bergmann, SSRL  
Gordon E Brown Jr, SSRL  
Serena DeBeer George, SSRL  
Philip A Heimann, LBNL  
Zahid Hussain, LBNL

Ingolf Lindau, SSRL (Chair)  
Anders Nilsson, SSRL  
Robert A Scott, University of Georgia  
David K Shuh, LBNL  
Glen A Waychunas, LBNL

## Organizing Committee

Uwe Bergmann, SSRL  
Gordon E Brown Jr, SSRL  
Stephanie Carlson, SSRL  
Serena DeBeer George, SSRL  
Britt Hedman, SSRL

Cathy Knotts, SSRL  
Ingolf Lindau, SSRL  
Piero Pianetta, SSRL  
Keith O Hodgson, SSRL

# XAFS13 Conference Overview

Gordon Brown – Stanford University and SSRL

The 13<sup>th</sup> International Conference on X-ray Absorption Fine Structure (XAFS) was held at Stanford University on July 10-14, 2006 and was attended by about 400 scientists representing 22 countries. Almost 100 oral presentations were made, including seven plenary lectures, and about 430 posters were presented during four poster sessions. The plenary lectures included two on recent advances in theoretical interpretations of X-ray Absorption Near Edge Structure (XANES) spectra, one on XAFS spectroscopic characterization of the manganese cluster in Photosystem II, one on the electronic and molecular structure of liquids as studied by picosecond XAFS, one on XAFS spectroscopy and x-ray fluorescence imaging studies of corrosion of glasses of different ages, including stained glasses from some of the great cathedrals of Europe, one on the application of XANES spectroscopy and photoemission electron microscopy to nanobiology, and one on the scientific career of Dale Sayers, one of the pioneers in XAFS spectroscopy who recently passed away. The scientific sessions included the Dale Sayers Symposium as well as the following disciplinary areas: (1) biology (active sites in isolated systems and *in-situ* imaging), (2) catalytic processes, (3) novel and unusual experimental methods, (4) modeling and data analysis approaches, (5) magnetic properties and systems, (6) time-resolved spectroscopy, (7) materials studies, (8) chemistry (processes and systems), (9) theory, calculations, and modeling, (10) environmental applications, (11) developments in XAS theory, (12) actinides in the environment, (13) *in-situ* XAS studies, (14) XAS and nanomaterials, and (15) biomedical XAS applications.

The conference co-chairs responsible for the overall organization of XAFS13 were Profs. Britt Hedman, Piero Pianetta, and Keith Hodgson of the Stanford Synchrotron Radiation Laboratory (SSRL). Conference organization and infrastructure needs were ably provided by a number of SSRL staff members, including Stephanie Carlson, Lisa Dunn, Cathy Knotts, Michelle Montalvo, Ann Mueller, Jennifer Peck, Jackie Robledo, Amy Rutherford, Todd Slater, and Michelle Steger. Financial support was provided by Stanford University, a number of US National Laboratories and international light sources [including the Advanced Photon Source (APS-Argonne National Lab), the Advanced Light Source (ALS-Lawrence Berkeley National Lab), the National Synchrotron Light Source (NSLS-Brookhaven National Laboratory), Stanford Synchrotron Radiation Laboratory (SSRL), Stanford Linear Accelerator Center (SLAC), Synchrotron Radiation Center (SRC), SOLEIL Synchrotron, Hamburger Synchrotronstrahlungslabor (HASYLAB), Berliner Elektronenspeicherring – Gesellschaft für Synchrotronstrahlung (BESSY), the Canadian Light Source (CLS), and the National Synchrotron Radiation Research Center (NSRRC)], as well as by the following commercial exhibitors: Brush-Wellman Electrofusion Products, Canberra, Kohzu America, Inc., VG Scienta, Inc., and XIA LLC.

There were a number of highlights at the XAFS13 Conference. One involved the tremendous advances being made in blending theory and experiment. An example of these advances is the recent oxygen K-edge XAS and X-ray Raman Scattering (XRS) studies of the structure of bulk water and the interpretation of these spectra using state-of-the-art density functional theory, as reported in the plenary lecture of Lars G.M. Pettersson of Stockholm University. As one conferee put it, it's amazing that a small pre-edge feature in the oxygen K-edge XAS spectrum of liquid water has turned the water community upside down in its understanding of the average structure of water, the most common solvent on Earth. Another example is the advance in understanding of pre-edge features of 3d-transition metal ions using multiplet theory, as discussed by Frank deGroot of the University of Utrecht. Also

highlighted by Vittal Yachandra of Lawrence Berkeley National Laboratory was the new understanding provided by XAFS spectroscopy of the photosynthetic water-oxidizing complex that contains a unique  $Mn_4Ca$  cluster. Another highlight involved discussion of new methods, particularly X-ray Raman Scattering, Resonance Inelastic X-ray Scattering (RIXS), quantitative structural analysis of matter using XANES spectroscopy, and ultrafast methods that allow time-resolved studies of matter at the picosecond time scale and below. Another area in which impressive advances have been made since XAFS12 was held in Malmö, Sweden in 2003 are new applications of XAFS and related methods in biology, chemistry, materials science (including magnetic and nanomaterials), environmental science, condensed matter physics, and medical science. The enormous growth in applications of XAFS spectroscopy in particular and synchrotron radiation methods in general to these and other areas of science and engineering was emphasized by discussions of a number of new synchrotron radiation sources, either nearing completion or in the final planning stages, including the Canadian Light Source (Saskatoon, Saskatchewan, Canada), Diamond Light Source (Didcot, Oxfordshire, UK), Synchrotron SOLEIL (Saint-Aubin, France), Australian Synchrotron (Boomerang 20) (Melbourne, Victoria, Australia), and the Spanish Light Source (ALBA) (Barcelona, Spain).

In addition to 20 thematic oral sessions and four general poster sessions, the XAFS13 Conference featured a special symposium honoring Dale Sayers, with talks by a number of his friends and scientific collaborators. Dale was one of the three pioneers of XAFS spectroscopy, all of whom have remained very active in its applications. At the time of his death in November 2005, Dale was actively pursuing new medical imaging methods using synchrotron radiation for applications in mammography. His two mentors, Farrell Lytle and Ed Stern, also remain very active, with Farrell using XAFS methods to study desert varnishes, and Ed Stern using XAFS to study ultrafast changes in thin metal films excited by lasers.

There were three awards presented in a ceremony the same afternoon. The Edward Stern International XAFS Society (IXS) Outstanding Achievement Award was given jointly to Calogero R. Natoli, INFN, Italy and John J. Rehr, University of Washington, USA in recognition of their fundamental contribution for the development of XAFS theory (presented by Ed Stern). The IXS Farrell Lytle Outstanding Young Scientist Award for Theory or Instrumentation was given to Pieter Glatzel, ESRF, France in recognition of his contribution in developing XAFS-related techniques such as x-ray emission spectroscopy, resonant and non-resonant x-ray scattering (presented by Farrell Lytle). The IXS Dale Sayers Young Scientist Award for Applications of XAFS was given to Jan-Dierk Grunwaldt, ETH, Switzerland in recognition of his contribution in the application of XAFS in catalysts and in the study of chemical reactions; this award was presented by Anne Sayers.

Overall, the XAFS13 Conference was a highly successful gathering of scientists who shared their new theoretical and experimental developments and a broad range of applications of XAFS spectroscopy. The large number of young scientists attending the meeting was impressive and bodes well for the future of this method and its applications. The presentations and lively discussions at XAFS13 made clear that since its introduction in 1971 by Sayers, Stern, and Lytle, XAFS spectroscopy has become a mature methodology with exciting applications in many areas of science and engineering. The 276 papers published in this proceedings volume attest to this statement. We look forward to the next international gathering of XAFS aficionados (XAFS14) in Camerino, Italy in Summer 2009.