

# X-RAY ABSORPTION FINE STRUCTURE

*Editor*

**S. SAMAR HASNAIN**

Daresbury Laboratory, Warrington, UK

Fachbereich Materialwissenschaft  
der Techn. Hochschule Darmstadt

Inv.-Nr.: 641



**ELLIS HORWOOD**

NEW YORK LONDON TORONTO SYDNEY TOKYO SINGAPORE

# Contents

Preface	xxiii
<b>I Fundamental aspects of EXAFS and XANES</b>	<b>1</b>
1 EXAFS - a critical review J.B. Pendry	3
2 Structure, many-body effects and their interrelation in inner-shell x-ray absorption spectra of condensed matter C.R. Natoli	6
3 Inelastic effects in x-ray spectroscopies: theories vs experiment J.J. Rehr	15
4 Relativistic effects in EXAFS and XANES R.J. Blake	21
5 Theory of high-energy electron energy loss spectra from solids T. Fujikawa	28
6 XANES of Cu(II) imidazole complexes and proteins in solution R.W. Strange, L.M. Murphy, P. Durham and S.S. Hasnain	32
7 Electronic information extracted from the polarization dependence of multiple scattering calculations Ph. Sainctavit and J. Petiau	35
8 Structural properties extracted from multiple-scattering calculations in silicon carbide nanocrystallites Ph. Sainctavit, J. Petiau, C. Laffon, A.-M. Flank and P. Lagarde	38
9 X-ray absorption near-edge structure calculations for small silicon oxide clusters D.L. Foulis and A.-M. Flank	41
10 Strength and width of the white lines in the K-absorption spectra of atomic 3d metals and in the L-absorption spectra of atomic rare earths U. Arp, G. Materlik, M. Meyer, M. Richter and B. Sonntag	44
11 2p x-ray absorption of 3d transition metal compounds F.M.F. de Groot, J.C. Fuggle, B.T. Thole and G.A. Sawatzky	48
12 Origin of multi-electronic satellites in the x-ray absorption spectra of 3d transition metal compounds G. van der Laan	51
13 XAFS analysis in the anharmonic limit; application to HI-T <sub>c</sub> superconductors and ferrosilicates J. Mustre de Leon, S.D. Conradson, A.R. Bishop, I.D. Raistrick and I. Batistic	54

14	Thermal vibration and melting from a local perspective E.A. Stern, P. Livins and Zhe Zhang	58
15	Does the $L_2/L_1$ comparison work well using the " $\pi$ approach"? The case of the cubic $BaF_2$ system J. Chaboy, J. Garcia, M. Sanchez del Rio and A. Marcelli	62
16	The fine structure of the atomic scattering factor tensor in anomalous dispersion region and the problem of determination of atomic ternary distribution function in amorphous media R.V. Vedrinskii, V.L. Kraizman, A.A. Novakovich and V.Sh. Machaviani	65
17	Electron scattering phase-shift and amplitude calculation method in XAFS-problem of complexes containing low-Z atoms R.V. Vedrinskii, L.A. Bugaev and V.M. Airapetian	68
18	Theoretical description of the 2-nd and more distant shells contribution into XAFS L.A. Bugaev, R.V. Vedrinskii and S.V. Permjakov	72
19	MSXAS: a system of programs for x-ray absorption spectra calculations using the multiple scattering approach M.F. Ruiz-Lopez, A. Filipponi, A. Di Cicco, T.A. Tyson, F. Bohr, M. Benfatto and C.R. Natoli	75
20	Freestyle EXAFS fit algorithm for systems with large disorder P. Kizler	78
21	EXAFS and MD simulation study of the RDF for small Cu particles W. Niemann, B.S. Clausen, L.B. Hansen, P. Stoltze and J.K. Nørskov	81
	<b>II X-ray magnetic circular dichroism</b>	<b>85</b>
22	Systematics of spin-dependent XANES G. Schütz	87
23	Magnetic circular dichroism studies with soft x-rays F. Sette, C.T. Chen, Y. Ma, S. Modesti and N.V. Smith	96
24	Quadrupole contribution to magnetic x-ray circular dichroism C. Brouder	106
25	Magnetic x-ray dichroism in $RFe_2$ laves phase ( $R = Ce, Gd, Lu$ ) J.P. Kappler, C. Brouder, G. Krill, F. Baudelet, E. Dartyge, A. Jucha and A. Fontaine	109
	<b>III Metals in biology</b>	<b>113</b>
26	EXAFS and crystallographic studies of metallo-proteins containing iron P.F. Lindley	115

- 27 XAFS study of the haemoglobin from a high altitude bird and its comparison with adult and foetal human haemoglobin 122  
J. Pant, A. Abbasi, Z.H. Zaidi, R.W. Strange, G.P. Diakun, G.R. Jones and S.S. Hasnain
- 28 EXAFS of soybean lipoxygenase-1: influence of lipid hydroperoxide activation and lyophilization on the structure of the soybean lipoxygenase non-heme iron active site 125  
L.M. Van der Heijdt, M.C. Feiters, S. Navaratnam, H.-F. Nolting, C. Hermes, G.A. Veldink and J.F.G. Vliegthart
- 29 X-ray absorption spectroscopy of diferrous and differic protein A of soluble methane monooxygenase from *Methylococcus capsulatus* (Bath) 128  
J.G. DeWitt, J.G. Bentsen, B. Hedman, A.C. Rosenzweig, J. Green, S. Pilkington, K.O. Hodgson, S.J. Lippard and H. Dalton
- 30 XAS investigations on the Fe(III)-Zn(II) center of purple acid phosphatase from red kidney beans 131  
S. Priggemeyer, P. Eggers-Borkenstein, A. Rompel, B. Krebs, G. Henkel, H. Witzel, M. Körner, H.-F. Nolting and C. Hermes
- 31 An extended x-ray absorption study of the iron core site of ferritin and haemosiderin 134  
P. Mackle, C.D. Garner, R.J. Ward and T.J. Peters
- 32 Native and chemically modified horse spleen apo-ferritin: an EXAFS study 139  
E. Chiancone, A. Desideri, S.S. Hasnain, S. Morante, S. Stefanini and R.W. Strange
- 33 XAFS studies of transferrins. An analysis using multiple scattering calculations 142  
M. Neu, R.W. Evans, P.F. Lindley, R.W. Strange and S.S. Hasnain
- 34 Polarized x-ray absorption spectroscopy of biological molecules 146  
J.E. Penner-Hahn, S. Wang and G.S. Waldo
- 35 XAFS studies on blue copper proteins: the effect of pH and oxidation state changes on the copper site 152  
L.M. Murphy, S.S. Hasnain, R.W. Strange, I. Harvey and W.J. Ingledeew
- 36 Reactivity of the laccase trinuclear copper active site with dioxygen: an x-ray absorption edge study 156  
G.O. Tan, J.L. Cole, E.K. Yang, K.O. Hodgson and E.I. Solomon
- 37 X-ray absorption spectroscopy on the metal binding sites of D-xylose isomerase 159  
H.-F. Nolting, C. Hermes, C. Sudfeldt, H. Witzel, B. Krebs and G. Henkel
- 38 X-ray absorption spectroscopic studies of the catalytic centres of Mo and V nitrogenases 162  
R.R. Eady, B.E. Smith, I. Harvey, J.M. Arber, C.D. Garner and S.S. Hasnain

39	Sulfur K and molybdenum L edge XAS of the nitrogenase iron-molybdenum cofactor under <i>in-situ</i> electrochemical control B. Hedman, P. Frank, B. J. Feldman, S.F. Gheller, F.A. Schultz, W.E. Newton and K.O. Hodgson	168
40	X-ray absorption spectroscopic studies of the binding of ligands to FeMoco I. Harvey, R.R. Eady, B.E. Smith, R.L. Richards, C.A. Gormal, C.D. Garner and S.S. Hasnain	171
41	Mn K-edge XANES spectroscopy for water-splitting Mn-enzyme in photosynthesis. High quality pre-edge features in the S <sub>1</sub> and S <sub>2</sub> states M. Kusunoki, T. Ono, M. Suzuki, A. Uehara, T. Matsushita, H. Oyanagi and Y. Inoue	174
42	An EXAFS study of the oxygen-evolving complex of photosystem II. A.R. Corrie, M.C.W. Evans, J.A.M. Hubbard, R.W. Strange and S.S. Hasnain	178
43	EXAFS studies of zinc model compounds: metal ion co-ordination in the DNA binding domain of the yeast transcriptional activator GAL4 J.F. Povey, G.P. Diakun, C.D. Garner, S.P. Wilson and E.D. Laue	181
44	EXAFS studies of Pt(II) antitumor drugs S. Benazeth, I. Ascone, H. Dexpert, B. Viossat, D. Nguyen-Huy	184
45	EXAFS studies of different centers of Ca <sup>2+</sup> -binding proteins A.F. Korystova, D.I. Kochubei, V.M. Shelestov and A.A. Vazina	187
	<b>IV Surfaces: SEXAFS, glancing angle, EXAFS and standing wave</b>	191
46	Enhanced anharmonicity in the low-Z adsorbate-metal surface interaction H. Rabus, D. Arvanitis, T. Lederer and K. Baberschke	193
47	Cs on Si(111) 7×7: A SEXAFS study D.R. Batchelor and D.A. King	200
48	Near noble metal vs. refractory metal silicide formation: Co/Si(100) vs. Mo/Si(100) - preparation dependence and interface structure U. Döbler, H.L. Meyerheim and A. Puschmann	203
49	XESD domination of the Si K-edge Cl <sup>+</sup> yield from Si(111)7×7-Cl D. Purdie, C.A. Muryn, N.S. Prakash, P.L. Wincott, G. Thornton and D.S.-L. Law	206
50	Pseudo-intramolecular behaviour of the Cl K-edge σ* resonance of Si(111)7×7-Cl and Si(100)2×1-Cl D. Purdie, C.A. Muryn, N.S. Prakash, K.G. Purcell, P.L. Wincott, G. Thornton and D.S.-L. Law	209

- 51 Local structure in laser and thermally annealed As-implanted silicon from total electron yield EXAFS 212  
J.L. Allain, J.R. Regnard, A. Bourret, G. Tourillon, A. Parisini and A. Armigliato
- 52 Fe and As K-edge EXAFS study of arsenate (AsO<sub>4</sub>)<sup>-3</sup> adsorption on "two-line" ferrihydrite 215  
G.A. Waychunas
- 53 An *ab initio* calculation of the near edge x-ray absorption fine structure of C<sub>2</sub> and O<sub>2</sub> chemisorbed on Ag(110) 218  
P.A. Stevens and T.H. Upton
- 54 SEXAFS of (2×1)O/Ag(110): missing-row reconstruction 223  
L. Becker, S. Aminpirooz, A. Schmalz, B. Hillert, M. Pedio and J. Haase
- 55 Surface reconstruction in (√17 × √17)R14° S/Cu(100) studied by surface XAFS 226  
Y. Kitajima, Y. Takata, T. Yokoyama, M. Yoshiki, M. Funabashi, T. Ohta and H. Kuroda
- 56 Underpotential-deposited Cu monolayer on Pt 229  
T.M. Hayes, W. Li, G. Liang, C.M. Lo, T.E. Furtak, E.A. Creek, P. Samanta and L. Wang
- 57 Glancing angle XAFS for the study of real surfaces 232  
G.N. Greaves, S. Pizzini, N.T. Barrett, K.J. Roberts and S. Kalbitzer
- 58 Ge/Si monolayer superlattices on Si(100) studied by surface-sensitive XAFS 238  
H. Oyanagi, T. Sakamoto, K. Sakamoto, H. Yakaguchi, Y. Kuwahara, T. Matsushita and T. Yao
- 59 XAFS studies of interactions at transition-metal/Al interfaces 242  
S.M. Heald and E.V. Barrera
- 60 Influence of annealing of Ni-C multilayer coatings using glancing angle fluorescence EXAFS 245  
G.E. van Dorssen, P. Mackle, E.J. Puik and H.A. Padmore
- 61 Surface relaxation of S and Cl adsorbed metals studied by surface EXAFS and the soft x-ray standing wave method 248  
T. Ohta
- 62 Soft x-ray standing wave absorption profiles of c(2×2)S/Ni(100) 254  
Y. Takata, T. Yokoyama, Y. Kitajima, M. Funabashi, H. Kuroda and T. Ohta
- 63 Surface EXAFS studies of sulfur adsorbed on stepped surface; S/Ni(7 9 11) 257  
H. Ishii, K. Asakura, Y. Kitajima, M. Funabashi, H. Namba, N. Kosugi, T. Ohta and H. Kuroda

64	EXAFS study of aqueous Co(II) sorption complexes on kaolinite and quartz surfaces P.A. O'Day, G.E. Brown, Jr., and G.A. Parks	260
65	In-situ EXAFS study of changes in Co(II) sorption complexes on $\gamma$ -Al <sub>2</sub> O <sub>3</sub> with increasing sorption densities C.J. Chisholm Brause, G.E. Brown, Jr., and G.A. Parks	263
66	In situ studies of potential dependent structural and distributional changes at electrochemical interfaces with x-rays H.D. Abruna, M. Bommarito and D. Acevedo	266
67	In-situ study of lithium electrochemical intercalation through x-ray absorption E. Prouzet, C. Cartier, A. Tranchant, R. Messina, F. Villain and H. Dexpert	276
68	An in-situ energy dispersive EXAFS study of the platinum fuel cell electrode S.E. Doyle, M.E. Herron, K.J. Roberts, J. Robinson and F.C. Walsh	279
	<b>V Glasses and covalent systems</b>	283
69	Applications of x-ray absorption and reflection in materials science B. Lengeler	285
70	An EXAFS study of amorphous Si(:Ar):H and Si:D A.M. Edwards, S.J. Gurman, M.C. Fairbanks and R.J. Newport	294
71	In-situ high-temperature x-ray absorption study of ferrous iron in orthosilicate crystals and liquids W.E. Jackson, G.E. Brown, Jr., G.A. Waychunas, J. Mustre de Leon, S.D. Conradson and J.M. Combes	298
72	Chemical ordering of Ge <sub>x</sub> SE <sub>100-x</sub> glasses: an x-ray absorption study W. Zhou, M. Paesler and D.E. Sayers	302
73	Polarized XANES analyses for arsenic pyramidal site environments in arsenic chalcogenide glasses J.M. Lee, M.A. Paesler and D.E. Sayers	305
74	EXAFS study of the structural environments of trace levels of Zr <sup>4+</sup> , Mo <sup>6+</sup> and U <sup>6+</sup> /U <sup>5+</sup> /U <sup>4+</sup> in silicate glass/melts systems F. Farges, C.W. Ponader and G.E. Brown, Jr.	309
75	X-ray absorption study of the local Ca environment in silicate glasses J.-M. Combes, G.E. Brown, Jr. and G.A. Waychunas	312
76	Densified SiO <sub>2</sub> glasses studied by XANES at the silicon K-edge I. Davoli, E. Paris, M. Benfatto, A. Gargano, S. Stizza and F. Seifert	315

- 77 Local structure of  $\text{CDS}_x\text{SE}_{1-x}$  compounds 319  
C. Levelut, A. Ramos and J. Petiau
- 78 An EXAFS study of germanium sulfide glasses 322  
P. Armand, A. Ibanez, E. Philippot, M. Ribes and H. Dexpert
- 79 Structural approach of the Ag-As-Se chalcogenide glasses: The  $\text{AsSe-Ag}_2\text{Se}$  line 325  
V. Mastelaro, S. Benazeth, H. Dexpert and J. Dugue
- 80 XANES study of lanthanum in glasses of the system  $\text{K}_2\text{O-SiO}_2\text{-La}_2\text{O}_3$  328  
E.M. Larson, A.J.G. Ellison, F.W. Lytle, A. Navrotsky, R.B. Greggor and J. Wong
- 81 XANES of  $\text{CdFeTe}$  and hypothetical zinc-blende  $\text{FeTe}$  332  
A. Kisiel, E. Burattini, P.M. Lee, G. Dalba and P. Fornasini
- 82 Ge and Ga-L x-ray absorption spectra in some semiconductors 337  
S. Naoé, K. Fukui, T. Matsukawa and T. Murata
- 83 Extended x-ray absorption fine structure study of  $\text{CrSe}_2$  340  
A.P. Deshpande
- 84 The local structure of IV-VI semiconductor alloys: lattice distortion and ferroelectric phase transitions 343  
B.A. Bunker, Z. Wang and Q. Islam
- 85 XANES of transition metal zinc-blende semiconductors 346  
D.A. McKeown
- 86 XANES study of valence fluctuation in  $\text{Sm}_{1-x}\text{Eu}_x\text{S}$  system 349  
R.K. Singhal and K.B. Garg
- 87 XAFS studies of metal drying additives in decorative paints 352  
I.S. Dring, R.J. Oldman, D. Walbridge and N.A.R. Falla
- 88 Thermochemical reduction effects in MgO doped with transition metals studied by EXAFS and XANES 356  
M. Sanchez del Rio, J. Garcia, J. Chaboy and R. Gonzalez
- 89 X-ray absorption study of metal coordination in Ni(II) and Cu(II) complexes 359  
B. Yu. Helmer, T.A. Lyubesnova, A.T. Shuvaev, V.L. Kraizman, A.A. Novakovich, A.S. Mirmilstein and A.A. Makarenko
- 90 XANES study of cobalt (II) complexes of some substituted imidazoles 362  
S.K. Joshi, B.D. Shrivastav and K.B. Pandeya

<b>VI Ionics and superconductors</b>	<b>365</b>
91 Disorder of Cu-O bonds in $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ , CuO and $\text{Cu}_2\text{O}$ A.N. Mansour, I. Talmy, D. Haught and R.D. Bardo	367
92 Polarization-dependent XAFS studies on a uniaxially oriented $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ superconductor H. Maruyama, H. Kimura, H. Maeda, T. Ishii, A. Koizumi and H. Yamazaki	370
93 Indication for a composite Cu 3d, 4s and O 2p state in high-Tc superconductors C.F.J. Flipse, G. van der Laan, A.L. Johnson and K. Kadowaki	373
94 X-ray absorption fine structure studies of $\text{Nd}_{2-x}\text{Ce}_x\text{CuO}_{4-y}$ H. Oyanagi, Y. Yokoyama, H. Yamaguchi, Y. Kuwahara, T. Katayama and Y. Nishihara	376
95 XAFS study on Tl-Ba-Ca-Cu-O superconductors H. Yamaguchi, H. Oyanagi, Y. Kuwahara, H. Ihara and Y. Syono	380
96 XANES study of Cu valence as function of oxygen doping in $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ K.B. Garg and K.V.R. Rao	383
97 Pr-L <sub>I-III</sub> near-edge study of 4f-hybridization in orthorhombic and tetragonal $\text{PrBa}_2\text{Cu}_3\text{O}_{7-x}$ G. Wortmann, P. Sladeczek, G. Stadermann, I. Felner and G. Kaindl	386
98 EXAFS and related studies of polymer electrolytes R.T. Edwards, R.J. Latham, R.G. Linford and R. Pyenburg	390
99 X-ray absorption studies on $\text{Li}_x\text{V}_2\text{O}_5$ electroformed compounds C. Cartier, M. Verdaguer, H. Dexpert, A. Tranchant and R. Messina	393
100 X-ray absorption study at the copper K-edge of Nasicon type phosphates E. Fargin, I. Bussereau, R. Olazcuaga, G. Le Flem, C. Cartier, H. Dexpert and M. Verdaguer	396
101 EXAFS study of indium tin oxide thin films Ph. Parent, H. Dexpert, G. Tourillon, J.M. Grimal and H. Harmand	399
102 Determination of the impurity position in photorefractive $\text{LiNbO}_3$ by EXAFS spectroscopy C. Prieto, C. Zaldo, P. Fessler, H. Dexpert, J.A. Sanz and E. Dieguez	402
103 Local structure of inorganic proton conducting materials on modification by ion-exchange and amorphisation D.J. Jones and J. Rozière	405
104 EXAFS study of thermal disorder in the non-superionic phases of AgI G. Dalba, D. Diop, P. Fornasini, P. Maistrelli and F. Rocca	408

105	Multiple scattering calculation of the XAS in the non-superionic phases of AgI S. Angeretti and M. Benfatto	411
106	EXAFS study of superionic conductor $\delta$ -Bi2O3 at high temperature K. Koto, A. Yoshiasa and S. Emura	414
107	Temperature dependent EXAFS-measurements on superionic conducting $\text{Pb}_{0.6}\text{Cd}_{0.4}\text{F}_2$ M.A. Denecke, Th. Lemke, W. Gunßer, I. Kosacki and W. Niemann	417
108	EXAFS studies of disorder in $\text{SrTiO}_3$ M. Joo, A. Edwards, Q. Islam and D. Sayers	420
109	Temperature-dependent EXAFS study on $\text{AgBr}_x\text{Cl}_{1-x}$ solid solutions T. Yokoyama, F. Takamatsu, K. Seki, K. Miyake, T. Tani and T. Ohta	423
110	Cerium $L_{\text{III}}$ absorption of plasma sprayed coatings: cerium valence state as function of the deposition temperature L. Alagna, G.M. Ingo, T. Proserpi and M.G. Simeone	426
111	EXAFS of alkali halides under high pressure and interatomic potentials J. Freund and R. Ingalls	429
112	Local structure around $\text{Cu}^+$ impurities in sodium chloride S. Emura, T. Murata, H. Maeda, M. Nomura, T. Moriga and A. Koizumi	432
113	Investigation of the structural environment around $\text{Cu}^{2+}$ in doped ammonium sulphate using EXAFS and standing waves D.R. Armstrong, D.A.H. Cunningham, K.J. Roberts and J.N. Sherwood	435
114	The rotation of oxygen octahedra in mixed oxygen perovskites B. Rechav and Y. Yacoby	438
115	High temperature XAFS study of perovskite-type $\text{La}_{1-x}\text{Sr}_x\text{CoO}_3$ ( $x = 0.2, 0.5$ ) H. Kageyama and N. Kamijo	442
	<b>VII Catalysts</b>	445
116	X-ray absorption spectroscopic studies of transition metal catalysts J.M. Corker, J. Evans, J.T. Gauntlett, H. Leach and J.F.W. Mosselmans	447
117	Ni EXAFS of Ni-MoS <sub>2</sub> hydrodesulphurization catalysts S.P.A. Louwers and R. Prins	455
118	An EXAFS study of the metal-promotor interface of a vanadia promoted rhodium catalyst in the precursor state A. Munoz-Paez and D.C. Koningsberger	458

- 119 Metal-promoted hydroformylation on a SiO<sub>2</sub>-supported Rh dimer: a direct observation of the structure change of active site in working conditions 461  
K. Asakura, K. Kitamura-Bando, Y. Iwasawa, H. Arakawa and K. Isobe
- 120 Local structure analysis of potential Rh organometallic catalysts by EXAFS 464  
J.A. Lopez, F.J. Lahoz, M.P. Garcia, J. Chaboy, J. Garcia and E. Burattini
- 121 Structural and chemical properties of Cu-based methanol catalysts 467  
B.S. Clausen, G. Steffensen, J. Hyldtoft, W. Niemann and H. Topsøe
- 122 XAFS study of Cu precipitates on microdefects in FZ-Si crystals 471  
T. Kitano, J. Mizuki and J. Matsui
- 123 Au-L<sub>3,2</sub> edge x-ray absorption studies of charge redistribution in Au-metalloid intermetallics 475  
T.K. Sham, Y.M. Yiu, M. Kuhn and S. McCuaig
- 124 X-ray absorption and Raman-UV/visible spectroscopic study of Au(III) complexes in chloride solutions: direct evidence for chlorine and oxychlorine complexes 478  
F. Farges, J.A. Peck and G.E. Brown, Jr.
- 125 EXAFS studies on homogeneous alkene oligomerisation catalysts 481  
J.M. Corker and J. Evans
- 126 XAFS study of FeCl<sub>3</sub> hydration and oxidation 484  
B.Yu. Helmer, T.A. Lybeznova, A.T. Shuvaev, V.L. Kraizman and A.A. Novakovich
- 127 Application of XAFS-spectroscopy to the structural characterization of new osmium catalysts 487  
A.T. Shuvaev, B.Yu. Helmer and Ph.M. Ovsjannikov
- 128 Structural characterisation of an amorphous intermetallic compound MgPdC<sub>x</sub>H<sub>y</sub> using x-ray absorption spectroscopy. EXAFS of PdC<sub>0.15</sub>, MgPd and Mg<sub>0.9</sub>Pd<sub>1.1</sub> 490  
D.J. Jones, J. Rozière, L.E. Aleandri, B. Bogdanovic and S.C. Hockett
- 129 In-situ EXAFS studies under high temperature and pressure of a Pt/Al<sub>2</sub>O<sub>3</sub> catalyst during reduction and hydrocarbon conversion 493  
N.S. Guyot-Sionnest, F. Villain, D. Bazin, H. Dexpert, F. Le Peltier, J. Lynch and J.P. Bournonville
- 130 EXAFS study of structural disorder in vanadium phosphate catalysts 496  
M. Lopez Granados, J.C. Conesa, M. Fernandez Garcia and C. Prieto
- 131 EXAFS characterization of calcined Ni-TiO<sub>2</sub>/SiO<sub>2</sub> catalysts prepared by hydrolysis of a Ni-allyl compound 499  
A. Fernandez, A. Caballero, M. Paneque, A.R. Gonzalez-Elipse, G. Munuera and E. Burattini

- 132 Structure and reactivity of ammonia synthesis catalysts derived from CeRu<sub>2</sub> precursors: an in situ XRD and XAS study  
A.P. Walker, T. Rayment, R.M. Lambert and R.J. Oldman 502
- 133 Thermal variation of the Ce L<sub>III</sub> edge in intermetallic compounds  
E. Beaurepaire, J.P. Kappler, J. Sereni, C. Godart and G. Krill 505
- 134 Cerium dioxide reduction and reoxidation followed by fast acquisition of XANES spectra  
F. Le Normand, C. Prieto, J. El Fallah, J. Majerus and O. Touret 508
- 135 Unusual iron atomic structure by EXAFS and XANES in Fe-Ru superlattices  
F. Baudalet, A. Fontaine, G. Tourillon, D. Guay, V. Dupuis, M. Maurer, M. Piecuch and M.F. Ravet 512
- 136 XANES/EXAFS of nickel-alumina catalysts  
P.J. McCluskey, D.S. Urch, N. Bausck and L.N. Mazalov 515
- 137 Structure of the molybdenum(V) oxalate and its surface compounds in Mo/Al<sub>2</sub>O<sub>3</sub> catalysts  
V.K. Fedorov, E.P. Degtyaryov, A.N. Startsev and O.V. Klimov 518
- 138 EXAFS study on the local structure of Co in an amorphous Co-Zr-Nb alloy  
Y. Uehara, N. Kamijo, H. Kageyama and T. Sakata 521
- 139 Structural study of Fe-Zr amorphous alloys prepared by mechanical alloying  
A. Corrias, G. Ennas, G. Licheri, G. Paschina, G. Vlaic and M. Magini 524
- 140 XAFS studies on local environment effect in Fe-Pt alloy system  
M. Fujita, H. Maruyama, H. Maeda, A. Koizumi and H. Yamazaki 527
- 141 An investigation of the structure of copper-rich precipitates in model  $\alpha$ -iron alloys  
S. Pizzini, K.J. Roberts, W.J. Phythian and C.A. English 530
- 142 X-ray absorption spectroscopic measurements of Ni 3d occupancy in NiCu binary alloys  
G. Meitzner, J.H. Sinfelt and D.A. Fischer 533
- 143 Local architecture around Al, Cu and Fe atoms in icosahedral AlCuFe quasicrystalline alloys  
A. Sadoc, A.M. Flank and P. Lagarde 536
- 144 XANES studies of rare earth metals and compounds  
N.K. Garg, K.K. Chaturvedi, G. Shah and S.N. Gupta 540
- 145 The local structure of Cu-Ta alloys synthesized by mechanical alloying  
K. Sakurai, Y. Yamada, M. Ito, C.H. Lee, T. Fukunaga and U. Mizutani 543
- 146 Time resolved XAS study of zeolite CuY during hydrogen treatment  
M. Hagedstein, S. Cunis, R. Frahm, W. Niemann, R. Piffer and P. Rabe 546

147	EXAFS and XANES studies of the environment of germanium and titanium in siliceous MFI-type zeolites A. Lopez, M.H. Tuilier, H. Kessler, J.L. Guth and J.M. Popa	549
148	Metal-atom substituted microporous materials - x-ray absorption spectroscopic studies P. Behrens, S. Abmann, J. Felzche, S. Vetter, G. Schulz-Ekloff, N.I. Jaeger and W. Niemann	552
149	Interference between the Fourier transform peaks of closely spaced shells: simulation of the Fourier transform for Fe <sub>2</sub> B M. Choi, J.I. Budnick, D.M. Pease, G.H. Hayes and J. Wong	556
150	An EXAFS study on mercury(II) halide complexes in dimethyl sulfoxide and pyridine solution I. Persson, J.E. Penner-Hahn and K.O. Hodgson	559
151	Zirconium complexes of "Axially prostereogenic" benzocoumarin-type lactones: EXAFS determination of the metal environment T. Ertel, S. Hückmann, H. Bertagnolli, G. Bringmann, C. Ewers, G. Erker, I. Hart and C. Sarter	562
152	EXAFS studies of some rhenium systems M.S. Islam	566
	<b>VIII Earth sciences</b>	571
153	EXAFS in earth sciences research C.M.B. Henderson, J.M. Charnock, G.R. Helz, S.C. Kohn, R.A.D. Patrick and D.J. Vaughan	573
154	EXAFS study of the non-cubic symmetry in garnet structure J. Dong and K. Lu	579
155	Comparative XAFS study of Na <sub>3</sub> Fe <sub>2</sub> (AsO <sub>4</sub> ) <sub>3</sub> and Na <sub>3</sub> Cr <sub>2</sub> (AsO <sub>4</sub> ) <sub>3</sub> garnets P. Berthet, J. Berthon, F. d'Yvoire and C. Masquelier	583
156	X-ray absorption investigation of vanadium binding sites in Maya and Arabian heavy petroleum residua G. Zhang and M.M. Boduszynski	587
	<b>IX Soft x-ray edges</b>	591
157	Soft x-ray spectroscopy in materials science P. Lagarde	593
158	Chlorine L-edge XANES investigations of alkali chlorides M. Kasrai, M.E. Fleet, G.M. Bancroft, D.G. Sutherland, K.H. Tan and J.M. Chen	601

159	XANES studies of some silicon compounds C. Laffon, A.M. Flank and P. Lagarde	604
160	Sulfur K-edge XAS studies of photographic materials T.A. Smith, J.G. DeWitt, B. Hedman and K.O. Hodgson	607
161	Determination of sulphur forms in coal by XAFS spectroscopy F.E. Huggins, G.P. Huffmann, S. Mitra and N. Shah	610
162	In-laboratory XAFS facility for low Z element: application to the local structure study of amorphous alumina N. Kamijo, H. Kageyama, K. Kawabata, K. Nishihagi, Y. Uehara and K. Taniguchi	613
163	EXAFS at the oxygen atoms in $\text{YBa}_2\text{Cu}_3\text{O}_7$ : A $K\alpha$ fluorescence yield study L. Tröger, D. Arvanitis, H. Rabus, K. Baberschke and B. Stritzker	616
164	Ultra soft x-ray fluorescence XAFS for in situ low Z materials characterization D.A. Fischer, G. Meitzner and J. Gland	619
	<b>X Experimental trends</b>	623
165	New developments in XAS experiments F.W. Lytle and R.B. Gregor	625
166	Exotic sources and new spectrometers for XAS studies with variable polarization P. Elleaume, J. Chavanne, X. Maréchal, J. Goulon, L. Braicovich and H. Emerich	634
167	Fluorescence XAFS array detectors for 0.3 - 20 keV S.P. Cramer, H. Kraner, S.J. George, L. Rogers, S. Rescia, V. Radeka, M. Yocum, J. Colaresi, O. Tench and O.C. Mullins	640
168	An ESRF beamline dedicated to polarization sensitive XAS at low excitation energies P. Elleaume, H. Emerich, J. Goulon, G. Marot, J. Sunini, L. Baricovich and C. Malgrange	646
169	Measuring XAFS of single crystal materials with electron detection K.H. Kim, W.T. Elam, E.F. Skelton, J.P. Kirland and R.A. Neiser	649
170	Optical EXAFS studies of single crystals of alkali halides T. Murata, S. Emura, T. Moriga, H. Maeda and M. Nomura	653
171	Exxon beamline X10C at NSLS, Brookhaven National Laboratory M. Sansone, G. Via, G. George, G. Meitzner and R. Hewitt	656
172	$L_{II,III}$ absorption edges of iron complexes using a multilayer/KAP two crystal monochromator C. Cartier and A.M. Flank	659

173	Absolute measurement of the energy of x-ray absorption edges for Cu, Ni, Zn and Yb J. Stümpel, P. Becker, S. Joksch, R. Frahm and G. Materlik	662
174	Performance of EXAFS stations at Photon Factory M. Nomura and A. Koyama	667
175	Noise and reproducible (non EXAFS) artefacts of an EXAFS station G. Kruizinga, M. Oversluizen, B.R. Dobson and D.C. Koningsberger	670
176	Photoacoustic EXAFS spectroscopy T. Masujima, T. Toyoda, H. Shiwaku and M. Ando	673
177	X-ray absorption spectroscopy of amorphous As <sub>2</sub> S <sub>3</sub> under hydrostatic pressure G. Pfeiffer, Q.T. Islam, A. Edwards, M.A. Paesler and D.E. Sayers	678
178	Possibilities of laboratory XAFS facilities Y. Udagawa	681
179	A new laboratory x-ray spectrometer for XAFS and XANES of light elements H. Wakita, S. Yamashita and K. Taniguchi	685
180	A laboratory bent crystal XAFS spectrometer S.N. Gupta, K.K. Chaturvedi and G. Shah	688
181	EXAFS studies of matrix isolated species I.R. Beattie, M.D. Spicer and N.A. Young	690
182	EXAFS study of solvophobic interactions of krypton in solutions of polar solvents D. Peter, A. Helmerich, H. Bertagnolli and R. Frahm	693
183	XANES studies of some silicon compounds C. Laffon, A.M. Flank and P. Lagarde	696
184	Characterisation of unstable species by x-ray absorption spectroscopy W. Levason, J.S. Ogden, M.D. Spicer and N.A. Young	699
185	Bonding microstructures in SiO clusters and in bulk by XAS A.M. Flank, R.C. Karnatak, C. Blancard, J.M. Esteva and P. Lagarde	702
	<b>XI EXAFS and related techniques</b>	<b>707</b>
186	XANES, anomalous small-angle scattering and fine scale composition fluctuations in amorphous Fe <sub>x</sub> Ge <sub>100-x</sub> films A. Bienenstock, R.D. Lorentz and M. Rice	709

187	The local structure of As-Te system glasses investigated by x-ray absorption spectroscopy and anomalous scattering Q. Ma, S. Benazeth and D. Raoux	715
188	Surface structure analysis of ZnTe by EAPFS R. Konishi, M. Arioka and H. Sasakura	719
189	X-ray Raman scattering from graphite: anisotropic effects K. Tohji, Y. Udagawa, T. Matsushita, M. Nomura and T. Ishikawa	722
190	Bragg reflectivity extended fine structure of germanium crystals I. Arcon, A. Kodre and M. Hribar	726
	<b>XII Time resolved EXAFS</b>	729
191	Quick XAFS: potentials and practical applications in materials science R. Frahm	731
192	Time resolved structural studies of nickel exchanged zeolite Y and nickel oxide using energy dispersive EXAFS G. Baker, C.R.A. Catlow, J.W. Couves, A.J. Dent, G. Derbyshire, G.N. Greaves and J.M. Thomas	738
193	Beamline instability-corrected, time-resolved data in dispersive x-ray absorption spectroscopy J.M. Lee, M.A. Paesler, D.E. Sayers and A. Fontaine	742
194	Microsecond time resolved XAFS P. Livins, D. Thiel, E.A. Stern, A. Lewis and M. Newville	745
	<b>XIII Standard and Criteria Workshops report</b>	749
195	Report on the International Workshops on Standards and Criteria in XAFS	751
	<b>Author Index</b>	771
	<b>Subject Index</b>	785