XAFS16 Proceedings

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New sources and new instrumentation

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A Modern Laboratory XAFS Cookbook
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Development of highly stable Bragg polychromator for energy dispersive XAFS
K Kato, T Irie, T Uruga, K Uera, and M Kawase
Filename: II_Tue_05_Kato_etal_Revised manuscript

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Advanced Methods

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Hydride phase formation in carbon supported palladium hydride nanoparticles by in situ EXAFS and XRD
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Filename: III_Mon_01_Bugaev_etal_Bugaev_PdH_XAFS16

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Filename: III_Mon_05_Amemiya_etal_kamemiya-final

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A Gainar, J S Stevens, E Suljoti, J Xiao, R Golnak, E F Aziz, and S L M Schroeder
Filename: III_Mon_10_Gainar_etal_revised (final)

XAFS studies of monodisperse Au nanoclusters formation in the etching process
L Yang, T Huang, W Liu, J Bao, Y Huang, Y Cao, T Yao, Z Sun, and S Wei
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Separation of Different Atomic Shells in EXAFS Spectrum Using the Regularization Method
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A Longo, C Lamberti, G Agostini, E Borfecchia, A Lazzarini, W Liu, F Giannici, G Portale, and E Groppo
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XAS and RIXS study of acetic acid and methyl formate in liquid
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Chemistry, catalysis, operando and time-resolved studies

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D Matsumura, Y Okajima, and Y Nishihata
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A M Abdel-Mageed, G Kučerová, A A El-Moemen, J Bansmann, D Widmann, and R J Behm
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Using combined XAS/DRIFTS to study CO/NO oxidation over Pt/Al_2O_3 catalysts
A M Gänzler, H Lichtenberg, A I Frenkel, M Casapu, A Boubnov, D Wang, and J-D Grunwaldt
Filename: IV_O_14_Gaenzler_etal

Chemical state of Ag in conducting bridge random access memory cells: a depth resolved X-ray absorption spectroscopy investigation
F d'Acapito, E Souchier, P Noe, P Blaise, M Bernard, and V Jousseaume
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Ex-situ and in-situ investigations of thermal anti-oxidation treatments of stainless steels by reflection mode EXAFS
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Dynamic transformation of small Ni particles during methanation of CO_2 under fluctuating reaction conditions monitored by *operando* X-ray absorption spectroscopy
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Local structure of iridium organometallic catalysts covalently bonded to carbon nanotubes
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XAS on Rh and Ir metal sites in post synthetically functionalized UiO-67 Zirconium MOFs
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In situ characterization of catalysts and membranes in a microchannel under high-temperature water gas shift reaction conditions
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Copper-oxide metalorganic nanocomposite: morphological and X-ray spectroscopy studies
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Structural characterization of bimetallic Pd-Cu vapor derived catalysts
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Energy dispersive-EXAFS for studying Pd nucleation at a liquid/liquid Interface
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Nb K- and L_3-edges XAFS study on the structure of supported Nb carbide catalyst
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Time-resolved study on dynamic chemical state conversion of SiO_2-supported Co species by means of dispersive XAFS technique
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Estimation of the catalytic centre in double metal cyanide catalysts by XAS
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Investigation of oxygen vacancies in CeO2/Pt system with synchrotron light techniques
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Flame made ceria supported noble metal catalysts for efficient H_2 production via the water gas shift reaction
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XAFS study on structural order in highly monodispersed thiol-stabilized Au nanoparticles
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Study of coordination environments around Pd and Pt in a Pd-core Pt-shell nanoparticle during heating
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PDMS embedded Ag clusters: Coalescence and cluster-matrix interaction
S Roese, D Engemann, S Hoffmann, K Latussek, C Sternemann, and H Hövel
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Structural analysis of NiO nanocluster catalysts on SiO_2 by using XAFS measurements
T Sasaki, N Ichikuni, T Hara, and S Shimazu
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Automated analysis of XANES: A feasibility study of Au reference compounds
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In situ observation of reduction kinetics and 2D-mapping of chemical state for heterogeneous reduction in iron-ore sinters
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Radionuclides, actinides, earth and environmental

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Probing changes in Hg(II) coordination during its bacterial uptake
S A Thomas, Q Ma, and J-F Gaillard
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An x-ray absorption spectroscopy study of Cd binding onto a halophilic archaeon
A R Showalter, J E S Szymanowski, J B Fein, and B A Bunker
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Absorption and Mobility of Cr and Zn in Soil in the Vicinity of Jordan River
M Harfouche, A M Ghrair, D M M Jaradat, G Aquilanti, R Jaber, A Aldrabee, and N Sawai
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Speciation of neptunium during sorption and diffusion in natural clay
T Reich, S Amayri, P J B Börner, J Drebert, D R Fröhlich, D Grolimund, and U Kaplan
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Metal (Hydr)oxides for the removal of Cr(VI) from drinking water: a XAFS study
F Pinakidou, E Kaprara, M Katsikini, E C Paloura, K Simeonidis, and M Mitrakas
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Structural properties of sodium-rich carbonate-silicate melts: An in-situ high-pressure EXAFS study on Y and Sr
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XAFS study of copper(II) diethylenetriamine complexes having different coordination geometries
A Gaur, W Klysubun, S K Joshi, B Soni, B D Shrivastava, J Prasad, and K Srivastava
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XAS signatures of Am(III) adsorbed onto magnetite and maghemite
N Finck, L Radulescu, D Schild, M Rothmeier, F Huber, J Lützenkirchen, T Rabung, F Heberling, M L Schlegel, K Dideriksen, S Nedel, and H Geckeis
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Aqueous U(VI) interaction with magnetite nanoparticles in a mixed flow reactor system: HR-XANES study
I Pidchenko, F Heberling, K O Kvashnina, N Finck, D Schild, E Bohnert, T Schäfer, J Rothe, H Geckeis, and T Vitova
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Fe, Ni and Zn speciation in airborne particulate matter
B Thiodjio Sendja, G Aquilanti, I Vassura, and M Giorgetti
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Chemical reactions of As complexation by glutathione: an XAFS study
M W Franco, I F Vasconcelos, L V Modolo, and F A R Barbosa
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The Ti environment in natural hibonite: XANES spectroscopy and computer modelling
A N Kravtsova, A V Soldatov, A M Walker, and A J Berry
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Characterization of fossil remains using XRF, XPS and XAFS spectroscopies
I M Zougrou, M Katsikini, F Pinakidou, M Brzhezinskaya, L Papadopoulou, E Vlachos, E Tsoukala, and E C Paloura
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Interpretation of the U L3-edge EXAFS in uranium dioxide using molecular dynamics and density functional theory simulations
D Bocharov, M Chollet, M Krack, J Bertsch, D Grolimund, M Martin, A Kuzmin, J Purans, and E Kotomin
Filename: V_Tue_01_Bocharov_etal_revised_final_ready for publication

Probing Covalency in the UO3 Polymorphs by U M4 edge HR-XANES
Y Podkovyrina, I Pidchenko, T Prüssmann, S Bahl, J Göttlicher, A Soldatov, and T Vitova
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Sorption mechanisms of metals to graphene oxide
A R Showalter, T A Duster, J E S Szymanowski, C Na, J B Fein, and B A Bunker
Filename: V_Tue_08_Showalter_etal_MLGO Conf Proc XAFS16 - revised final

Local structures of Ca, Ti and Fe in meteorite fusion crusts
T Tobase, A Yoshiasa, T Hiratoko, H Hongu, H Isobe, A Nakatsuka, H Arima, and K Sugiyama
Filename: V_Tue_10_Tobase_etal_Tobase XAFS16 2015 proceedings Journal of Physics2

Valence determination of rare earth elements in lanthanide silicates by L3-XANES spectroscopy
A N Kravtsova, A A Guda, J Goettlicher, A V Soldatov, V K Taroev, A A Kashaev, L F Suvorova, and V L Tauson
Filename: V_Tue_12 Kravtsova_final_revised

Weathering and precipitation after meteorite impact of Ni, Cr, Fe, Ca and Mn in K-T boundary clays from Stevns Klint
Y Miyano, A Yoshiasa, T Tobase, H Isobe, H Hongu, M Okube, A Nakatsuka, and K Sugiyama
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Fission products behaviour in UO2 submitted to nuclear severe accident conditions
E Geiger, R Bès, P Martin, Y Pontillon, P L Solari, and M Salome
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Micro and conventional XAFS study of incinerated Cr-rich tannery sludge
F Pinakidou, M Katsikini, S Varitis, P Kavouras, and E C Paloura
Filename: V_Tue_16_Pinakidou_etal_revised

Materials Science

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Structural and magnetic properties of nanoclusters formed in III-V semiconductors
K Lawniczak-Jablonska, A Wolska, and M T Klepka
Filename: VI_KN_23_LawniczakJablonska_etal_nano_wydz_proceedings_corMyD

Local dynamics and phase transition in quantum paraelectric $SrTiO_3$ studied by Ti K-edge x-ray absorption spectroscopy
A Anspoks, J Timoshenko, J Purans, F Rocca, V Trepakov, A Dejneka, and M Itoh
Filename: VI_O_09_Anspoks_SrTiO3_v1d

EXAFS study of the structural properties of In and In + C implanted Ge
R Feng, F Kremer, D J Sprouster, S Mirzaei, S Decoster, C J Glover, S A Medling, S P Russo, and M C Ridgway
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Subtle local structural variations in oxygen deficient niobium germanate thin film glasses as revealed by x-ray absorption spectroscopy
M A Sahiner, A Nabizadeh, D Rivella, L Cerqueira, J Hachlica, R Morea, J Gonzalo, and J C Woicik
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Soft x-ray absorption spectroscopy on Co doped ZnO: structural distortions and electronic structure
I A Kowalik, E Guziewicz, M Godlewski, and D Arvanitis
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Structural characterisation of Fe_2O_3 nanoparticles
M Hagelstein, D Vinga Szabó, S Schlabach, P Masala, M Scavini, M Coduri, and C Ferrero
Filename: VI_O_22_Hagelstein_et_al_RevisionMyD

Structure analyses of Cu nanoclusters in the soft magnetic $Fe_{85.2}Si_1B_9P_4Cu_{0.8}$ alloy by XAFS and fcc cluster model
M Matsuura, M Nishijima, K Konno, H Ofuchi, K Takenaka, and A Makino
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F Hu, S Zhang, Z Pan, W Yan, Q Liu, T Yao, and S Wei
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Combined spectroscopic study on the growth mechanism of Diphosphine-stabilized Gold Nanoclusters
J Bao, L Yang, W Liu, Y Huang, T Huang, Y Cao, T Yao, Z Sun, and S Wei
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Investigation of Prussian Blue Analogs by XMCD at the K-edge of transition metals
A Bordage, L Nataf, F Baudelet, and A Bleuzen
Filename: VI_Mon_14_Bordage_etal_bordage_revised-manuscript

Silver nanoparticles in silicate glass prepared by UV laser irradiation: dependences of size and atomic structure of particles upon irradiation parameters
M Dubiel, M Heinz, V V Srabionyan, V V Pryadchenko, L A Avakyan, Ya V Zubavichus, J Meinertz, J Ihlemann, and L A Bugaev
Filename: VI_Mon_19_Dubiel_etal_Dubiel_final_form

Co K-edge magnetic circular dichroism across the spin state transition in $LaCoO_3$ single crystal
V Efimov, A Ignatov, I O Troyanchuk, V V Sikolenko, A. Rogalev, F. Wilhelm, E Efimova, S I Tiutiunnikov, D Karpinsky, V Kriventsov, E Yakimchuk, S Molodtsov,
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A Y Geondzhian, A A Yaroslavtsev, P A Alekseev, R V Chernikov, B R Gaynanov, F Baudelet, L Nataf, and A P Menushenkov
Filename: VI_Mon_25_Geondzhian_etal_JPCS_25_Geondzhian_v1

High local disorder in $Tb_2Hf_2O_7$ pyrochlore oxide nanocrystals
V A Kabanova, V V Popov, Ya V Zubavichus, E S Kulik, A A Yaroslavtsev, R V Chernikov, and A P Menushenkov
Filename: VI_Mon_29_Kabanova_etal_JPCS_Kabanova_final

Thermally activated decomposition of (Ga,Mn)As thin layer at medium temperature post growth annealing
Y Melikhov, P Konstantynov, J Domagala, J Sadowski, M Chernyshova, T Wojciechowski, Y Syryanyy, and I N Demchenko
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XAFS study on the impact of local structure on electrochemical performance for Co_3O_4 nanowire arrays
S. Jiang, W Cheng, J He, J Huang, Q Liu, Y Jiang, and S Wei
Filename: VI_Tue_03_Jiang_etal_XAFS16_manuscript_VI_Tue_03_Jiang_etal_R

Grazing incidence X-ray absorption characterization of amorphous Zn-Sn-O thin film
S L Moffitt, Q Ma, D B Buchholz, R P H Chang, M J Bedzyk, and T O Mason
Filename: VI_Tue_08_Moffitt_etal_XAFS16-VI_Tue_08_Moffitt-revised

Importance of local structural distortions in magnetocaloric effect in Mn based antiperovskites
K R Priolkar, E T Dias, G Aquilanti, Ö Çakir, M Acet, and A K Nigam
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EXAFS and X-ray diffraction study of $LaCoO_3$ across the spin-state transition
V V Sikolenko, I O Troyanchuk, V V Efimov, E A Efimova, S I Tiutiunnikov, D V Karpinsky, S Pascarelli, O Zaharko , A Ignatov, D Aquilanti, A G Selutin, A N Shmakov, and D Prabhakaran
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Dependence of the Jahn-Teller distortion in $LaMn_{1-x}Sc_xO_3$ on the isovalent Mn-site substitution
G Subías, V Cuartero, J Blasco, J García, C Meneghini, and G Aquilanti
Filename: VI_Tue_21_Subias_etal_JPCS_LaMnScO3_final

Oxidation-resistive copper nanoparticles: photoreduction synthesis and their oxidation state measurements by XAFS and HRTEM
H Tanaka, T Aoki, M Yonemura, M Miyagawa, and K Okumura
Filename: VI_Tue_22_Tanaka_etal_d-RevisedManuscript(CameraReady)

Temperature dependence of Zr and Ti K-edge XANES spectra for para-and ferro-electric perovskite-type $PbZrO_3$, $PbTiO_3$and $BaTiO_3$
A Yoshiasa, T Nakatani, T Hiratoko, T Tobase, A Nakatsuka, M Okube, H Arima, and K Sugiyama
Filename: VI_Tue_30_Yoshiasa_etal_YoshiasaXAFS16 2015 proceedings Journal of Physics ver3_Introjustified

Pressure-induced insulator-to-metal transition in α-$SnWO_4$
A Kuzmin, A Anspoks, A Kalinko, J Timoshenko, R Kalendarev, L Nataf, F Baudelet, T Irifune, and P Roy
Filename: VI_Tue_33_Kuzmin_etal_revised_final

Polarization-dependent DANES study on vertically-aligned ZnO nanorods
C Sun, C In Park, Z Jin, I Hwang, S M Heald, and S Wook Han
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Energy-related materials

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In situ XANES & XRD Study of interphasial reaction between uncharged Li_2FeSiO_4 cathode and $LiPF_6$-based electrolyte
Z Arthur, H C Chiu, X Lu, N Chen, V Emond, G P Demopoulos, and D T Jiang
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A XAFS study of the local environment and reactivity of Pt-sites in functionalized UiO-67 MOFs
E Borfecchia, S Øien, S Svelle, L Mino, L Braglia, G Agostini, E Gallo, K A Lomachenko, S Bordiga, A A Guda, M A Soldatov, A V Soldatov, U Olsbye, K P Lillerud, and C Lamberti
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Simulation of the EXAFS and Raman spectra of $InxGa_{1-x}N$ utilizing the equation of motion routine of FEFF8
M Katsikini, F Pinakidou, E C Paloura, J Arvanitidis, S Ves, U Reinholz, E Papadomanolaki, and E Iliopoulos
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Structural and electronic studies of metal hexacyanoferrates based cathodes for Li rechargeable batteries
M Giorgetti, A Mignani, G Aquilanti, P Conti, M Fehse, and L Stievano

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XAFS study on structure-activity correlations of α-$Co(OH)_2$ nanosheets water oxidation catalysts
J Huang, Q Liu, T Yao, Z Pan, and S Wei
Filename: VII_Mon_02_Huang_etal_RevisedVersionJHHuang-xafs16 manuscript

Investigation on Electrochemical Property of AB/Al_2O_3-coated Li-excess Mn-based Layered Oxides
H Kobayashi, K Takada, Y Arachi, T Okumura, M Shikano, and H Nitani
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Local structure modification in lithium rich layered Li-Mn-O cathode material
M Giorgetti, D Wang, G Aquilanti, D Buchholz, and S Passerini
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Fe local structure in Pt-free nitrogen-modified carbon based electrocatalysts: XAFS study
A Witkowska, G Giuli, M Renzi, S Marzorati, W Yiming, F Nobili, and M Longhi
Filename: VII_Tue_10_Witkowska-paper

Structural phase transitions in ionic conductor Bi_2O_3 by temperature dependent XPD and XAS
Y Zhu, P An, M Yu, A Marcelli, Y Liu, T Hu, and W Xu
Filename: VII_Tue_13_Zhu_etal_JPCSformat_Bi2O3-final
Supporting Information: VII_Tue_13_Zhu_etal_Bi2O3-suppl .docx

Soft Matter and biology

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NEXAFS and XPS of p-Aminobenzoic Acid Polymorphs: The Influence of Local Environment
J S Stevens, A Gainar, C Jaye, D A Fischer, and S L M Schroeder
Filename: VIII_O_06_Stevens_etal_polymorph paper_2_final

Biomimetic mono- and dinuclear Ni(I) and Ni(II) complexes studied by X-ray absorption and emission spectroscopy and quantum chemical calculations
N Schuth, S Mebs, H Gehring, B Horn, P Holze, R Kositzki, P Schrapers, C Limberg, and M Haumann
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Unveiling the complex network of interactions in Ionic Liquids: a combined EXAFS and Molecular Dynamics approach
A Serva, V Migliorati, A Lapi, and P D'Angelo
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NEXAFS Chemical State and Bond Lengths of p-Aminobenzoic Acid in Solution and Solid State
J S Stevens, A Gainar, E Suljoti, J Xiao, R Golnak, E F Aziz, and S L M Schroeder
Filename: VIII_Mon_05_Stevens_etal_pH bond length paper_1_final

EXAFS characterisation of metal bonding in highly luminescent, UV stable, water-soluble and biocompatible lanthanide complexes

A. Kalyakina, V. Utochnikova, A. Trigub, Y. Zubavichus, N. Kuzmina, and S. Bräse
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Local atomic structure and oxidation processes of Cu(I) binding site in amyloid beta peptide: XAS Study
M A Kremennaya, M A Soldatov, V A Stretsov, and A V Soldatov
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Microscopy, beamlines, applications, cultural heritage

Time resolved XANES illustrates a substrate-mediated redox process in Prussian blue cultural heritage materials
C Gervais, M-A Lanquille, G Moretti, and S Réguer
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A microchannel confocal examination of arsenic speciation and distribution in *Bufo americanus*
M M Nearing, I Koch, R A Gordon, and K J Reimer
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New data evaluation procedure including advanced background subtraction for radiography using the example of insect mandibles
S Mangold, T van de Kamp, and R Steininger
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SPring-8 BL36XU: Catalytic Reaction Dynamics for Fuel Cells
O Sekizawa, T Uruga, Y Takagi, K Nitta, K Kato, H Tanida, K Uesugi, M Hoshino, E Ikenaga, K Takeshita, S Takahashi, M Sano, H Aoyagi, A Watanabe, N Nariyama, H Ohashi, H Yumoto, T Koyama, Y Senba, T Takeuchi, Y Furukawa, T Ohata, T Matsushita, Y Ishizawa, T Kudo, H Kimura, H Yamazaki, T Tanaka, T Bizen, T Seike, S Goto, H Ohno, M Takata, H Kitamura, T Ishikawa, M Tada, T Yokoyama, and Y Iwasawa
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Inhomogeneous distribution of chemical species in lithium nickel oxide cathode of lithium ion battery
T Uenoyama, R Miyahara, M Katayama, and Y Inada
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Study of the relation between Mg content and dissolution kinetics of natural lime stone using µXRF, µXRD and µXAS
H S Grunwaldt, A Zimina, J Göttlicher, R Steinniger, and J D Grunwaldt
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Industrial Session

XAFS characterization of industrial catalysts: *in situ* study of phase transformation of nickel sulfide
J Wang, Z Jia, Q Wang, S Zhao, Z Xu, W Yang, and A I Frenkel
Filename: IS_O_06_Wang_etal

XAFS beam lines at Aichi Synchrotron Radiation Center dedicated to industrial use
Y Takeda
Filename: IS_O_09_Takeda

Workshop "Data acquisition, treatment, storage-quality assurance in XAFS spectroscopy"

XAFS data acquisition with 2D-detectors: Transmission mode XAFS and grazing incidence EXAFS spectroscopy
D Lützenkirchen-Hecht, J-C Gasse, R Bögel, R Wagner, and R Frahm
Filename: WS_01_DESY_Luetzenkirchen_etal

XAFS Data Interchange: A single spectrum XAFS data file format
B. Ravel and M. Newville
Filename: WS_02_DESY_Ravel_Newvile

ROCK: the new Quick-EXAFS beamline at SOLEIL
V Briois, C La Fontaine, S Belin, L Barthe, Th Moreno, V Pinty, A Carcy, R Girardot, and E Fonda
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