

07:30	Registration				07:30
08:30	Welcome session B. Bunker, IXAS President; D. Löhle, KIT Vice President; F. Mentrup, Mayor of the City of Karlsruhe; B. Murphy, KFS Vice President; J.-D. Grunwaldt, XAFS16 Chair				08:30
09:20	General announcements				09:20
09:30	III-PL-01 Serena de Beer X-ray emission spectroscopic studies of biological catalysis	C. Heske			09:30
10:10			Coffee break		10:10
10:40	Time-resolved and ultrafast R. Frahm, A. Rochet	From hard to soft X-rays G. Vanko, W. Caliebe	Fundamental theory A. di Cicco, C. Jacob	Environmental I R. Dähn, A. Manceau	10:40
10:50	IV-O-01 Y. Li Origin of giant electrostriction in Gd doped ceria revealed by differential QEXAFS	III-O-01 P. Miedema State-dependent fluorescence through the Coulomb exchange	I-KN-01 J.J. Kas Advances in the theory and calculation of many-body effects in x-ray spectra	V-O-01 S.A. Thomas Coordination environment of Hg(II) bound to E. coli in the presence and absence of organic ligands: influence of metabolic activity	10:50
11:10	IV-O-02 S. Gu Quick-scanning system update at SSRF XAFS experimental station	III-O-02 T. Kroll Extracting Electronic Structure. Information from 1s2p RIXS and L-edge XAS of Transition Metal Complexes	I-O-02 F.D. Vila Dynamic structural disorder and reactivity in supported metal nanocatalysts	V-O-02 A.R. Showalter An X-ray absorption spectroscopy study of Cd binding onto a halophilic archaeon	11:10
11:30	IV-O-03 M. Chergui Pico- and Femtosecond X-ray absorption study of electron localization in photoexcited TiO2 nanoparticles	III-O-03 P. Glatzel Orbital mixing and multiplet effects in the K absorption pre-edges of TiO2 and Mn2O3	I-O-03 J. Rehr Efficient Bethe-Salpeter equation calculations of x-ray spectra of large systems	V-O-03 M. Harfouche Absorption and Mobility of Cr and Zn in Soil in the Vicinity of Jordan River	11:30
11:50	IV-O-04 J. Just Nucleation and Growth Kinetics of Multinary Nanocrystals by Quick Extended X-ray Absorption Fine Structure	III-KN-04 S. Huotari Non-resonant X-ray Raman scattering spectroscopy	I-O-04 B. Ravel FEFF85EXAFS: open source theoretical standards for EXAFS analysis	V-O-04 E. Montarges-Pelletier Zn K-edge XAFS for the study of river material reactivity towards metals	11:50
12:10					12:10
12:20			Lunch break		12:20
13:20	Catalysis & Novel methods A. Jentys, V. Briois	Nano-analysis and applications K. Ławniczak-Jabłońska	Data analysis B. Ravel, M. Newville	Actinides & Radionuclides I M. Denecke, J. Rothe	13:20
13:30	IV-KN-05 C. Lamberti		I-O-05 H. Ikemoto miXAFS: A Program for X-ray Absorption Fine Structure Data Analysis	V-KN-05 S. Conradson	13:30
13:40	Local environment and electronic structure of active sites in Cu-SSZ-13 deNOx catalyst under reaction conditions	VI-O-01 M. Staniuk Tracking of the changes during nucleation and growth of nanoparticles in solution – MCR-ALS analysis of time-resolved XANES data	I-O-06 M.U. Delgado-Jaime Analysis of X-ray spectra by fitting Multiplet Simulations to experimental data	Novel Structural Chemistry – and More – from Actinide XAFS	13:40
14:00	IV-O-06 B. Liu In-situ 2p3d resonant x-ray emission spectroscopy of Co/CNT Fischer-Tropsch catalysts	VI-O-02 T. Petit Interfacial water on nanodiamonds in colloidal dispersions probed by transmission X-ray absorption spectroscopy	I-O-07 K. Hatada EXAFS analysis using the new Graphical User Interface of the GNXAS suite of programs	V-O-06 T. Vitova High energy resolution XANES as a tool for electronic and geometric structural investigations of actinide materials	14:00
14:20	IV-O-07 R. Kopelent Identification of active and spectator species during low-temperature CO oxidation on a ceria-based catalyst using in situ time-resolved resonant X-ray emission spectroscopy	VI-O-03 H.W.P. Carvalho In situ XAS uncovering the mechanisms of thermal stabilization of polymer-clay nanocomposites	I-O-08 J. Timoshenko Disappearance of correlations in the atom motion upon hydrogen intercalation into ReO3 lattice: in-situ EXAFS study, deciphered by a novel reverse Monte Carlo / evolutionary algorithm approach	V-O-07 M.I. Boyanov Biological and abiotic factors affecting the solid-phase speciation of U(VI) following reduction of aqueous U(VI)	14:20
14:40	IV-O-08 P.P. Wells XAFS Investigations of MoOx/Fe2O3 based systems	VI-O-04 S. Mirzaei Characterizing the structural properties of the NPs formed by ion implantation in LPCVD and PECVD Si3N4 using XAS	I-O-09 A.A. Guda Efficient multicore parallelization of the finite difference method for x-ray absorption spectroscopy in the FDMNES code	V-O-08 V.A. Samson Identifying the "Unidentified": Crud Deposits from Swiss Pressurized Water Reactor Analyzed by Multi-Edge micro-X-ray Absorption Spectroscopy, micro-XRD and Complementary Chemical Imaging	14:40
15:00	IV-O-09 L. Lukashuk Investigation of preferential CO oxidation over Co3O4 and CeO2-Co3O4 by operando X-ray absorption spectroscopy	VI-O-05 A. Konashuk Advanced ultralow-k organosilicate glasses: NEXAFS study	I-O-10 X. Junquig X-ray absorption spectra of graphene and graphene oxide by Full Potential Multiple Scattering calculations with self-consistent potential	V-O-09 T. Reich Speciation of neptunium during sorption and diffusion in natural clay	15:00
15:20					15:20

	Catalysis & Noble metal clusters O. Safonova, W. Grünert	Nanostructures, Ferroelectrics to metal-organic frameworks D. Batchelor	Instrumentation beamlines P. Kappen, V. Briois	Biology S. de Beer, M. Haumann	
15:50					15:50
16:00	IV-O-10 D. Matsumura Precise observation of structural change of Pd nanoparticles during surface adsorption and catalytic reaction	VI-KN-06 F. Rocca Negative thermal expansion of ScF ₃ : an EXAFS study at the Scandium K-edge from 10 K up to 1100 K	II-KN-01 M. Newville Upgraded X-ray Spectroscopy Microprobe Beamline 13-ID-E of the Advanced Photon Source	VIII-KN-01 W.S. Chu Progress in XANES ab initio calculations of complex metalloenzymes with two metal centers	16:00
16:20	IV-O-11 X. Pan Confinement effects of carbon nanotubes on catalysis	VI-O-07 H. Wahab Identification of carbon bonds in graphene oxide using soft x-ray reflectometry	II-O-02 O. Mathon X-ray Absorption Spectroscopy under Extremes	VIII-O-02 M. Haumann Metal-hydride intermediates in FeFe and NiFe hydrogenase enzymes detected and characterized by XAS/XES and DFT	16:20
16:40	IV-O-12 T. Uchiyama Mechanochemical preparation and local structural analysis of Pd-LaFeO ₃ solid solutions by Pd K- and L3-edge X-ray absorption spectroscopy	VI-O-08 M. Rovezzi High-resolution x-ray absorption and emission spectroscopy study of Mn incorporation in Al _x Ga _{1-x} N hetero-structures	II-O-03 T. Uruga Quick XAFS system with millisecond time resolution	VIII-O-03 J. Kowalska Insights into the electronic structure of iron atoms in FeMo cofactor of nitrogenase and related models	16:40
17:00	IV-O-13 A.M. Abdel-Mageed Geometric and electronic structure of Au on Au/CeO ₂ catalysts during the CO oxidation: Deactivation by reaction induced particle growth	VI-O-09 A. Anspoks Local dynamics and phase transition in quantum paraelectric SrTiO ₃ studied by Ti K-edge x-ray absorption spectroscopy	II-O-04 W. Caliebe High-Flux EXAFS Beamline P64 at PETRAIII	VIII-O-04 F. Stellato Zn(II)/Cu(II) cross-coordination to Ab peptides can modulate the peptide aggregation propensity. A XAS structural study	17:00
17:20	IV-O-14 A. Gänzler Operando structure-activity correlations in applied catalytic systems: Oscillatory CO oxidation in exhaust gas catalysts	VI-O-10 M. Rangus XAS study of structural dynamics induced by heating and hydration of Ca-terephthalate metal-organic framework	II-O-05 O. Müller The new QEXAFS monochromator, detection and data acquisition system at the SuperXAS beamline (SLS) for EXAFS spectroscopy with 15 ms time resolution	VIII-O-05 B. Pollakowski Characterization of surface contaminants of medical devices	17:20
17:40	Evening break, transition to poster session				17:40
18:00	Poster session I				18:00
19:30					19:30

Topic color code

General
I. Theory and Modelling, Data analysis
II. New sources and new instrumentation
III. Advanced Methods
IV. Chemistry, catalysis, operando and time-resolved studies
V. Radionuclides, actinides, earth and environmental
VI. Materials Science
VIII. Soft Matter and biology