

Program



XAFS16

16th International Conference on X-ray Absorption Fine Structure

23–28 August 2015, Karlsruhe | ITCP/ANKA/INE

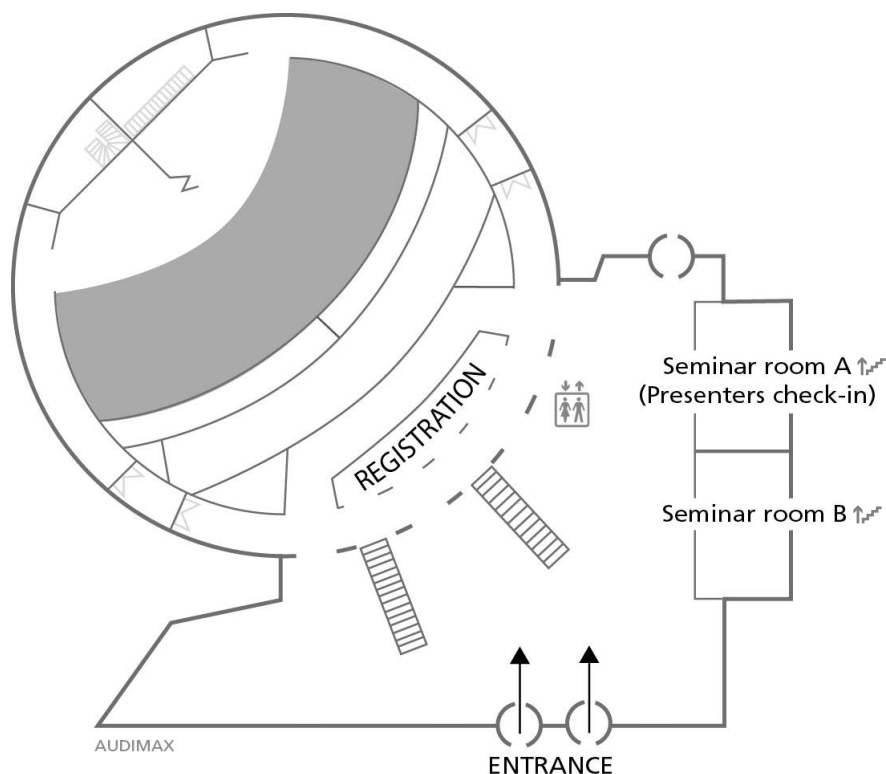


Conference program overview | UTC + 01:00 Amsterdam, Berlin, Bern, Rome, Stockholm, Vienna

Sunday 23 August 2015 16:00–20:00	16:00–19:00 Registration 18:00–20:00 Welcome party
Monday 24 August 2015 07:30–19:30	07:30 Registration 08:30–10:10 Plenary session: welcome general announcements plenary talk 10:10 Coffee break, after parallel sessions 10:40–17:40 Parallel session, lunch & coffee breaks 18:00–19:30 1 st poster session (with refreshments)
Tuesday 25 August 2015 08:30–19:30	08:30–10:10 Plenary session: plenary talks conference picture general announcements 10:10 Coffee break, after parallel sessions 10:40–17:40 Parallel sessions, lunch & coffee breaks 18:00–19:30 2 nd poster session (with refreshments)
Wednesday 26 August 2015 08:30–19:10	08:30–10:10 Plenary session: plenary talks IXAS & CXAFS/IUCr presentations 10:10 Coffee break, after parallel sessions 10:40–12:40 Parallel sessions after lunch: excursions 14:00–19:10 h
Thursday 27 August 2015 08:30–23:00	08:30–10:00 Plenary session: plenary talks / general announcements 10:00 Coffee break, after parallel sessions 10:20–17:00 Parallel sessions, lunch & coffee breaks 18:00–19:00 Center for Art and Media (ZKM) guided tour 19:00–23:00 Conference banquet at ZKM
Friday 28 August 2015 08:30–18:00	08:30–09:50 Plenary session: plenary talks / IXAS awards ceremony / general announcements 09:50 Coffee break, after parallel sessions 10:20–12:30 Parallel sessions 13:40–15:00 Plenary session: plenary talk / XAFS17 presentation / closing remarks 15:00–18:00 ANKA tour 18:00 Sino-German Workshop on Catalysis and Membranes

General Information

The registration desk is located in the Audimax:



Opening hours

■ Sunday:	16:00 – 19:00
■ Monday:	07:30 – 17:30
■ Tuesday:	08:00 – 17:30
■ Wednesday:	08:00 – 14:00
■ Thursday:	08:00 – 14:00
■ Friday:	08:00 – 14:00

Internet Access / WiFi

All registered participants will receive personalized guest account data upon check-in to connect mobile devices like smart phones, tablets and laptops to a wireless network for free access to internet services. All participants are obliged to adhere to the WiFi terms of use!

Help Desk

+49 (0) 721 / 608 47390

Emergency Number

112 (Emergency) / 110 (Police)

Taxi

+49 (0) 721 / 160 200 (Taxi-Ruf Karlsruhe)

+49 (0) 721 / 94 41 44 (Taxi-Funk-Zentrale Karlsruhe)

Photos/Videos

It is prohibited to take photos and/or videos in all buildings.



16:00	Registration		16:00
		Audi max	
	Welcome party		18:00
19:00			
20:00			20:00

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
VII. Energy-related materials
VIII. Soft Matter and biology
IX. Microscopy, beamlines, applications, cultural heritage
XFEL, Industriesession

Monday, August 24

07:30	Registration				07:30
08:30	Welcome session B. Bunker, IXAS President; D. Löhe, 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(IV) 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	Coffee break				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		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	Audimax B	II-KN-01 M. Newville Upgraded X-ray Spectroscopy Microprobe Beamline 13-ID-E of the Advanced Photon Source	Neue Chemie	VIII-KN-01 W.S. Chu Progress in XANES ab initio calculations of complex metalloenzymes with two metal centers	15:50		
16:00	IV-O-10 D. Matsumura Precise observation of structural change of Pd nanoparticles during surface adsorption and catalytic reaction	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	16:00		
16:20	IV-O-11 X. Pan Confinement effects of carbon nanotubes on catalysis	VI-O-08 M. Rovezzi High-resolution x-ray absorption and emission spectroscopy study of Mn incorporation in AlxGa1-xN 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	16:20		
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-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	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-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	17:00		
17:20	IV-O-14 A. Gänzler Operando structure-activity correlations in applied catalytic systems: Oscillatory CO oxidation in exhaust gas catalysts						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

08:30	II-PL-02 Anders Nilsson Ultrafast X-ray Spectroscopic Probing of Catalytic Surface Chemical Reactions using LCLS	F. de Groot	Audi max		08:30	
09:10	V-PL-03 Alain Manceau Emerging applications of high-resolution XANES spectroscopy in environmental science	A. Vögelin			09:10	
09:50	Conference picture and general announcements			09:50		
10:10	Coffee break			10:10		
10:30	Environmental II A. Manceau, J. Göttlicher	Operando and time-resolved G. Aquilanti, J. Purans	Advanced XAS Techniques I P. Glatzel, S. Huotari	Surfaces and interfaces D. Lützenkirchen-Hecht, H. Abe	Soft X-Ray XAFS A. Nilsson	10:30
10:40	V-KN-10 A. Voegelin	VI-O-11 A.D. Winter	III-KN-05 M. Nachttegaal	IV-KN-15 K. Asakura	XFEL-01 S. Schreck	10:40
10:50	Exploring the formation and structural diversity of Fe(III)-precipitates in aquatic systems using XAS	Thermo-mechanical behaviour of EVA/CNT composites studied through in situ NEXAFS spectroscopy	Time-resolved x-ray absorption and emission spectroscopies to determine the structure of the catalytic active site	Polarization dependent total reflection fluorescence XAFS and the control of metal structures on oxide surfaces	Implications of adding the dimension of time to science with X-rays	10:50
11:10	V-O-11 D. Cabaret Probing the 3d states of Fe in goethite using Al K-edge XANES spectroscopy	VI-O-12 T. Yao Time-resolved XAFS in kinetic formation and transition mechanism of nanoclusters and nanocrystals	III-O-06 J.-C. Gasse Yoneda-XAFS experiments with X-ray area detectors	IV-O-16 H.L. Meyerheim XAFS study of the local structure of iron on the (0001) surface of the topological insulator Bi2Se3	XFEL-02 P. Wernet Orbital-specific mapping of chemical dynamics	11:10
11:30	V-O-12 F. Pinakidou Metal (Hydr)oxides for the removal of Cr(VI) from drinking water: a XAFS study	VI-O-13 D. Degler Operando X-ray absorption spectroscopy: A key technique to understand the structure-function-relationship of noble metal doped gas sensing materials	III-O-07 G. van der Laan Probing the magnetization dynamics of spin valve systems using x-detected ferromagnetic resonance	IV-O-17 N.I. Verbitskiy Atomically precise semiconductor-graphene interfaces by Ge intercalation	XFEL-03 R. Carley Ultrafast generation of magnetic ordering in a first order phase transition in FeRh	11:30
11:50	V-O-13 R. Dähn X-ray microspectroscopic investigations of heavy metal uptake by argillaceous rocks	VI-O-14 T. Asanova Energy-dispersive XAFS and PXRD study of (NH4)2[OsCl6] thermolysis	III-O-08 C.T. Chantler The quality of X-ray Absorption Fine Structure measurements by Transmission for dilute systems, using the Hybrid Technique	IV-O-18 F. d'Acapito The Role Of Ag and Sb Ions In The Resistive Switching Mechanism Of Conductive Bridging Random Access Memories	XFEL-04 M. Beye Stimulating soft X-ray emission from condensed matter	11:50
12:10						12:10

	Earth and extreme conditions A. Vögelin, R. Dähn	In situ and operando studies A. Leon, F. Scheiba	XES + RIXS H. Carvalho, M. Nachttegaal	Surfaces and electrocatalysis K. Asakura, S.L. Schroeder	Hard X-Ray XAFS C. Bressler	
13:30	V-KN-14 Y. Ping	VII-KN-01 D. Asakura	III-KN-09 M. Bauer	IV-O-19 D. Lützenkirchen-Hecht	XFEL-05 K. Gaffney	13:30
13:40	XAFS in high-energy-density matter: solid iron up to 560GPa	Electrochemical operando soft x-ray emission spectroscopy for Li-ion-battery electrodes	Homogeneous catalysis and high resolution hard X-ray absorption and emission spectroscopy	Ex-situ and in-situ investigations of thermal anti-oxidation treatments of Cr-Ni steels by reflection mode EXAFS	Probing chemical reaction dynamics with atomic resolution and specificity using ultrafast x-ray spectroscopy	13:40
14:00	V-O-15 J. Pohlenz Structural Properties of Sodium-Rich Carbonate-Silicate Melts: An In-situ High-Pressure EXAFS Study on Y and Sr	VII-O-02 M. Tromp Operando XAS Characterization of LIS Batteries	III-O-10 S. Mebs Abrupt vs. gradual spin-cross-over in classic Fe(II) and Fe(III) compounds analyzed by high-resolution XAS/XES and DFT	IV-O-20 M.-H. Chu In situ X-ray absorption spectroscopy characterization of the incipient growth of ZnO thin films by atomic layer deposition	XFEL-06 G. Vankó Tracking light-induced ultrafast transformations of transition metal complexes	14:00
14:20	V-O-16 M.J. Ward Large area – high spatial resolution iron XANES mapping of impact melt-bearing breccias	VII-O-03 Z. Arthur In situ XAS/XRD Study of Li ₂ FeSiO ₄ as LIB Cathode Material	III-O-11 A. Bordage In situ site-selective K-edge XAS: A powerful probe of the transformation of mixed-valence compounds	IV-O-21 K.K. Bando In situ XAFS and XRD observation during a preparation process of an electroluminescent Tb doped alumina film	XFEL-07 T. Katayama Developments for time-resolved X-ray spectroscopies using X-ray Free Electron Lasers at SACLA	14:20
14:40	V-O-17 N. Thammajak Discovering effect of radiation interaction on color of freshwater cultured pearls	VII-O-04 K. Aziz-Lange In-situ techniques for soft X-ray spectroscopy on catalytic and electrochemical systems	III-O-12 M. al Samarai Redox sensitivity of cobalt in the CoMoS and CoNiMoS HDS catalyst: a Resonant Inelastic X-ray Scattering study	IV-O-22 L.A. Bugaev Atomic structure of PtCu nanoparticles in PtCu/C catalysts prepared by simultaneous and sequential deposition of components on carbon support	XFEL-08 Y. Uemura Femto to Picosecond Transient States of a Photoexcited WO ₃ Photocatalyst	14:40
15:00		VII-O-05 G. Aquilanti Operando XAS study of Li-S batteries		IV-O-23 L. Zhang EXAFS-A Powerful Tool to Determine the Structure of Active Species in Single-atom Catalysts	XFEL-09 D. Zhu Development in Ultrafast X-ray Spectroscopy at the X-ray Pump Probe Instrument of the LCLS	15:00
15:20	Coffee break					15:20

15:40	Earth & Radionuclides T. Reich, M. Boyanov	Nanostructures & Coordination chemistry C. Roth, Y.-L. Soo	Implanted atoms and particles F. Boscherini	Session reserved for special topics	XFEL XAFS Applications W. Gawelda	
15:50	V-O-18 K. Kvashnina Recent progress in high energy resolution X-ray spectroscopy of actinides	VII-O-06 M. Marcus Asymmetric pathways in the electrochemical conversion reaction of NiO as battery electrode with high storage capacity	VI-O-15 A. Figueroa Local structure and bonding of magnetic dopants in Bi ₂ Se ₃ and Bi ₂ Te ₃ topological insulator thin films	To be announced on short notice	X-Ray Spectroscopy at XFELs – Present and Future	15:40
16:10	V-O-19 B. Mishra Using X-ray Raman to Study Soil Carbon Biogeochemistry	VII-O-07 A. Zitolo XAS spectroscopic fingerprint of the active site in non-precious metal electrocatalysts for PEM fuel cells	VI-O-16 R. Feng EXAFS study on the structural properties of In and In + C implanted Ge			15:50
16:30	V-O-20 A. Gaur XAFS study of copper(II) diethylenetriamine complexes having different coordination geometries	VII-O-08 E. Borfecchia A XAS study of the local environment and reactivity of Pt-sites in functionalized UiO-67 MOFs	VI-O-17 M.A. Sahiner Subtle local structural variations in oxygen deficient niobium germanate thin film glasses as revealed by x-ray absorption spectroscopy			16:10
16:50	V-O-21 M. Vespa X-Ray Absorption Spectroscopic analyses of stable Fe-phases in aged cements	VII-O-09 W. Szczerba On the electronic structure and coordination geometry of iron based metallo-supramolecular coordination polyelectrolytes in working electrochromic devices	VI-O-18 I.A. Kowalik Soft x-ray absorption spectroscopy on Atomic Layer Deposition grown ZnO films			16:30
17:10					XFEL-12 Y. Kayser RIXS spectroscopy at hard XFELs using non-monochromatized SASE pulses	16:50
17:20					XFEL-13 M. Harmand Matter under extreme conditions probed with ultrafast XANES on FEL facilities	17:10
					XFEL-close out C. Bressler/W. Gawelda	17:20

Evening break, transition to poster session

18:00	Poster session II					18:00
19:30						19:30

Topic color code

General
III. Advanced Methods
IV. Chemistry, catalysis, operando and time-resolved studies
V. Radionuclides, actinides, earth and environmental
VI. Materials Science
VII. Energy-related materials
XFEL, Industrial Symposia

08:30	IV-PL-04 Simon Bare In situ XAFS: An Industrial Perspective	J.-D. Grunwaldt	Audi max	08:30		
09:10	IX-PL-05 Jennifer Mass Fading Old Masters and post-Impressionists: XANES Methodologies for the Preservation of Iconic Paintings	R. Gordon		09:10		
09:50	IXAS presentation	B. Bunker, P. Glatzel		09:50		
10:00	Presentation of CXAFS/IUCr	C. Chantler		10:00		
10:10	Coffee break			10:10		
	Microscopy & cultural heritage R. Gordon, J. Hormes	Operando spectroscopy X. Bao, J.A. van Bokhoven	Nanotechnology & Magnetism G. van der Laan	Instrumentation detectors C. Glover, L. O’Ryan		
10:40	IX-KN-01 P. Gilbert	IV-O-24 J. Radnik In situ XAS investigations of the butane oligomerization under industrially relevant conditions	VI-O-19 C. Guglieri Real-time structural study of the synthesis of ZnO nanoparticles capped with dodecanethiol molecules	II-KN-06 C. Fiorini	10:40	
10:50	PEEM and Pearls			New trends and challenges for detectors and electronics for XAFS	10:50	
11:10	IX-O-02 C. Gervais Time resolved XANES illustrates a substrate-mediated redox process in Prussian blue cultural heritage materials	IV-O-25 M. Steib On the role of metal-support interactions on the structural and catalytic properties during CH4 reforming reactions		VI-O-20 E. Fonda Structure and stability of self assembled metallic nanowires in CeO2 or SrTiO3	II-O-07 S.M. Heald Looking for the Limits of Fluorescence Detection of XAFS	11:10
11:30	IX-O-03 L. Monaco Synchrotron X-ray spectromicroscopy for the study of the photo-redox alteration process of chrome yellow pigments: towards safer illumination conditions and original color reconstruction of Van Gogh paintings	IV-O-26 B. Mutz Methanation of CO2: Structural response of Ni-based catalysts under fluctuating reaction conditions unraveled by operando XAS		VI-O-21 A.V. Soldatov Determination of the 3D Local Atomic and Electronic Structure of Nanoparticles by Combining of X-Ray Absorption and Computer Modeling	II-O-08 V. Marian Electrically-cooled HPGe detector for advanced x-ray spectroscopy and imaging	11:30
11:50	IX-O-04 E. Willneff Near Edge X-Ray Absorption Fine Structure (NEXAFS) Imaging of Artists’ Acrylic Paint Films	IV-O-27 A.I. Frenkel Structural and charge heterogeneities in supported nanoscale metal clusters	VI-O-22 M. Hagelstein Structural characterisation of Fe2O3 nanoparticles	II-O-09 J. Uhlig Microcalorimeters for time-resolved and other photon-starved x-ray spectroscopies	11:50	
12:10	IX-O-05 P.-J. Sabbe Chemical imaging of heritage metal surfaces with X-ray-excited optical microscopy	IV-KN-28 L. van Haandel Hydrotreating catalyst activation under industrial conditions	VI-KN-23 K. Ławniczak-Jabłońska Structural and magnetic properties of nanoclusters formed in III-V semiconductors	II-O-10 L.A. Martin-Montoya Data reduction for the 100 pixel Ge detector for XAS	12:10	
12:30					12:30	
12:40					12:40	
Lunch break						
14:00	Excursions				14:00	
19:10					19:10	

Topic color code

General
II. New sources and new instrumentation
IV. Chemistry, catalysis, operando and time-resolved studies
VI. Materials Science
IX. Microscopy, beamlines, applications, cultural heritage

08:30	V-PL-06 Philippe Martin Application of HERFD and in situ XAS to the investigation of oxide nuclear fuel and fission product behavior	M. Denecke	Audi max		08:30	
09:10	I-PL-07 Peter Blaha Electron-hole interactions in theoretical XAFS calculations	P. Glatzel		09:10		
09:50	General announcements			09:50		
10:00	Coffee break			10:00		
10:20	Actinides & Radionuclides II S. Conradson, T. Vitova	L-edge theory F. de Groot, P. Blaha	Devices and applications D. Haskel	Advanced in situ C. Chantler, C. Lamberti	Industrial symposium I A.I. Frenkel, K. Kvashnina, M. Casapu	
10:30	V-O-22 S.M. Butorin Ground state character in high-resolution x-ray absorption at M, N and O edges of actinides	I-KN-11 M. Haverkort Ab initio methods for core level spectroscopy - excitons, resonances and band excitations in time and frequency domain	VI-O-24 M. Matsuura Structure analyses of Cu clusters and precipitated α -Fe during nanocrystallization of soft magnetic Fe85.2Si1B9P4Cu0.8 alloys by XAFS	III-O-13 S. Baier Lithographically fabricated silicon microreactor for in situ characterization of heterogeneous catalysts	IS-Introduction A.I. Frenkel	
10:40					IS-O-01 T. Hyde Study of Industrial Catalysts by X-Ray Adsorption Spectroscopy	
11:00		V-O-23 D. Prieur Electronic and structural changes induced by the incorporation of aliovalent cation in UO2	I-O-12 H. Ikeno Development of the Ab-Initio Multiplet Approach for K pre-edge and L2,3-edge RIXS in Transition Metal Compounds	VI-O-25 S. Lafuerza LuFe2O4: a potential charge-ordering driven multiferroic studied by XAS at the Fe and O K-edges	III-O-14 O. Hirsch Atomic and electronic structure of La2O2CO3 on the basis of X-ray absorption and emission spectroscopy and the reactivity of La2O2CO3 films towards CO2	IS-O-02 P. Albers Applications of synchrotron radiation and neutron scattering in industrial catalyst research
11:20		V-O-24 N. Finck EXAFS signatures of trivalent actinides uptake by green rust and magnetite	I-O-13 I. Josefsson Modeling x-ray spectra of metal complexes from first principles	VI-O-26 R. Schepper High energy resolution X-ray absorption and emission spectroscopy for the investigation of spin crossover processes	III-O-15 V. Briois Study of SnO2 nanoparticles genesis using combined time-resolved Raman and Quick-XAS spectroscopies	IS-O-03 C. Tyrsted
11:30	V-O-25 G. Creff Actinides interaction with human bone: speciation and accumulation mechanisms	I-O-14 M. Guo Simulations of iron K pre-edge X-ray absorption spectra using the core restricted active space method	VI-O-27 D. Grandjean Structural characterization of highly luminescent molecular silver clusters embedded in LTA zeolites using combined Ag K-edge XEOL and transmission-detected EXAFS	III-O-16 E.K. Gibson A combined XAFS/DRIFTS study of AuPd nanoparticle restructuring	The nitrate-nitrite equilibrium: a key step in the NH3-SCR mechanism over Cu-CHA type catalysts	
11:40					IS-O-04 Y. Nagai Study of automotive catalysts for emission control by X-ray absorption spectrometry	
12:00		V-O-26 I. Pidchenko U Redox State and Speciation of U In Contact with Magnetite Nanoparticles: High Resolution XANES, EXAFS, XPS and TEM Study	I-O-15 M. Hunault Tracking the signature of low symmetry environments in the XAS K pre-edge	VI-KN-28 T. Miyayana XAFS study on luminescent Ag zeolites	III-KN-17 S. Best X-ray Spectroelectrochemistry – Valuable use of sample?	
12:20						
12:30						
Lunch break						
	Nanostructures A. Soldatov, M. Giorgetti	Applied theory J. Rehr, M. Haverkort	Atoms and solvation A. Goldbach, M. Ronning	Microscopy application C.G. Schroer, U. Boesenberg	Industrial symposium II A.I. Frenkel, K. Kvashnina, M. Casapu	
13:40	VII-KN-10 S. Price In situ XAS of electrochemical systems	I-KN-16 P. D'Angelo The structure of liquids: an insight from XAFS and Molecular Dynamics	IV-O-29 S.-Y. Chang Evidence for a Strongly Bound Solvent Molecules: XANES and EXAFS of Aqueous Au(III) Cyanide	IX-KN-06 K. Janssens XAFS and species-specific imaging: new and old combinations for elucidating natural alteration reactions in pigmented materials	IS-O-05 A. Kroner Industrial Research on Catalysis at Diamond Light Source	
13:50					IS-O-06 J. Wang XAFS characterization of Industrial catalysts for metal-containing molecular sieves	
14:10		VII-O-11 M. Katsikini Simulation of the EXAFS and Raman spectra of InxGa1-xN enabling the equation of motion routine of FEFF8	I-O-17 R. Nemausat Experimental and ab initio study of phonon effects in X-ray Absorption Near-Edge Structure spectroscopy	IV-O-30 J. Szlachetko Two-photon absorption using off-resonant excitation with ultrashort X-ray pulses	IX-O-07 R. Gordon A microchannel confocal examination of arsenic speciation and distribution in Bufo americanu	
14:30		VII-O-12 H. Kim X-ray absorption study of the newly observed reaction mechanism of mesoporous SnO2 electrode for the next generation Li-ion battery	I-O-18 P. Krüger Calculation of L23-edge spectra of K, Ca and Ti compounds with multichannel multiple scattering theory	IV-O-31 S.A. Thomas An X-ray absorption spectroscopy study of the molecular structure of aqueous Hg(II)-EDTA	IX-O-08 F. Mosselmans Micro X-ray imaging of single catalyst particles under operating conditions	IS-O-07 C. Tardivat
14:40	VII-O-13 N. Lock Copper doped TiO2 characterized by X-ray absorption spectroscopy, total scattering and powder diffraction	I-O-19 I.E. Brumboui The influence of oxygen adsorption on the O1s XPS and NEXAFS spectra of the C60 derivative PC60BM	IV-O-32 S. Bartlett Stopped-Flow Freeze-Quench EXAFS: A New Method to Investigate In-Situ Homogeneous Catalysis	IX-O-09 J. Hormes Synchrotron radiation based X-ray absorption and X-ray fluorescence for art and cultural heritage: opportunities and pitfalls	In-situ XAFS studies of Pt/CeO2 oxidation catalysts	
14:50						
15:10						
		Coffee break				15:10

					Industrial symposium III A.I. Frenkel, K. Kvashnina, M. Casapu	
15:30	RIXS and gas release E. Umbach, L. Weinhardt	Advanced XAS Techniques II E. Aziz, T. Kroll	Phase transitions and theory H. Ebert, C. Schmitz-Antoniak	Microscopy instrumentation G. Falkenberg, A. Rosenhahn	IS-O-08 T. Honma	15:30
15:40	VII-O-14 L. Amidani Probing with RIXS plasmonic-generated charges in TiO2/Au for photocatalysis	III-O-18 C. Jansing Investigation of the Natural X-Ray Birefringence of Graphene by Polarization Spectroscopy	VI-O-29 F. Goillou XANES/XMCD study at K-edges of the ferromagnetic transition of MnFe(P,Si,B) magnetocaloric materials	IX-O-10 P. Tack A novel approach towards full-field emission mode micro-XANES spectroscopy	Current status of Industrial Utilization of XAFS at Spring-8	15:40
16:00	VII-O-15 C. Sternemann Thermally induced hydrogen desorption in magnesium and calcium borohydrides	III-O-19 K.A. Lomachenko HERFD XANES and RIXS spectroscopies: probing the electronic structure of osmium complexes	VI-O-30 N.M. Souza-Neto Probing 5f-6d electronic hybridization in Uranium compounds with L2,3 edge x-ray magnetic circular dichroism	IX-O-11 S. Mangold Newest advances with radiography at the ANKA-XAS using the example of insect mandibles	IS-O-09 Y. Takeda XAFS beam lines at Aichi SR Center dedicated to industrial use	16:00
16:20	VII-O-16 M. Nishibori Relationship between O2 desorption property and bulk/local structure of La-Sr-Co-Fe perovskite-type oxide in atmospheres with varying oxygen partial pressure	III-O-20 R. Boada X-ray spectroscopy study of gas adsorption in metal organic frameworks	VI-O-31 O. Sips Intuitive view on the magnetic dipole term Tz occurring in the XMCD sum rules	IX-O-12 L. Lühl The Confocal XRF Setup for Chemical Speciation: Reconstruction Procedure for Confocal XANES and Three-Dimensional Chemical Mapping	IS-O-10 A.I. Frenkel, K. Kvashnina	16:20
16:30						16:30
16:40	VII-O-17 I. Pankin Phase transition in Mn(BH4)2 upon heating: combined XAS, XRD and DFT study	III-O-21 S. Zhao Correlative use of operando XAS and operando TEM for studies of structural dynamics of catalyst	VI-O-32 N. Mas Ab-initio calculation of K-edge XMCD and XNCD spectra	IX-O-13 O. Sekizawa SPRING-8 BL36XU: Catalytic Reaction Dynamics for Fuel Cells	Roundtable discussion	16:40
17:00						17:00
Individual transfer to Center for Art and Media (ZKM)						
18:00	Center for Art and Media (ZKM) tour					18:00
19:00						19:00
Dinner						
Poster awards						
Official end 23:00						
23:00						23:00

Topic color code

General
I. Theory and Modelling, Data analysis
III. Advanced Methods
IV. Chemistry, catalysis, operando and time-resolved studies
V. Radionuclides, actinides, earth and environmental
VI. Materials Science
VII. Energy-related materials
IX. Microscopy, beamlines, applications, cultural heritage
XFEL, Industrial Symposia

Friday, August 28

08:30	VI-PL-08 Hao Tjeng Fe3O4 thin films: epitaxial growth and properties	V. Saile		08:30
09:10	IXAS awards Dale Sayers Award, Ferrel Lytle Award, Ed Stern Award	B. Bunker, P. Glatzel		09:10
09:40	General announcements			09:40
09:50	Coffee break			09:50
	Nanomagnetism & Multiferroics D. Haskel, A. Juhin	Biology and soft matter P. D'Angelo, H. Harris	Catalysis J.-D. Grunwaldt, M. Tromp	Instrumentation & experimental set-up S. Diaz-Moreno, T. Hutwelker
10:20	VI-KN-33 C. Schmitz-Antoniak	VIII-O-06 J.S. Stevens	IV-KN-33 X. Bao	II-KN-11 G. Seidler
10:30	XMCD on Fe-based nanoparticles: Two examples of theory and experiment complementing one another	NEXAFS and XPS of p-Aminobenzoic Acid Polymorphs	XAS study on confined nanocatalysis	The Modern Laboratory XAFS Cookbook
10:50	VI-O-34 A. Juhin	VIII-O-07 F. Jalilehvand	IV-O-34 V. Marchionni	II-O-12 C. La Fontaine
	Hard X-ray RIXS-MCD, a magnetic spectroscopy for in situ characterization of nanoparticles and their internal structure	Lead(II) binding to thiol-containing molecules of biological interest in aqueous solution	Influence of CO on methane oxidation of TWC by combined spectroscopic and modulation approach	ROCK: the Quick-EXAFS beamline at SOLEIL
11:10	VI-O-35 H. Wende	VIII-O-08 O. Polozhentsev	IV-O-35 W. Grünert	II-O-13 K. Witte
	Electric in-plane polarization in multiferroic CoFe2O4/BaTiO3 nanocomposite tuned by magnetic fields	Synthesis and characterization of pure and rare earth doped Fe3O4 magnetic nanoparticles	Surface Alloy or Ion-Metal Interaction? How XRD and in-situ XAFS Help Understanding the Promotion of Cu by Zn in Methanol Synthesis Catalysts	XANES measurements with laboratory setups in the soft X-ray region using a Laser Produced Plasma Source
11:30	VI-O-36 V. Cuartero	VIII-O-09 J. Czapla-Masztafiak	IV-O-36 Y. Joly	II-O-14 N. Pilet
	Local spin state study on Co-doped multiferroic TbMnO3 by Kb X-ray emission spectroscopy	Investigating DNA radiation damage mechanisms using X-ray Absorption Spectroscopy (XAS)	Study of morphology and hydrogen coverage of nanometric platinum particles	NanoXAS - Combining Scanning Probe and X-Ray Microscopy for Nanoanalytics
11:50	VI-O-37 N. Daffe	VIII-O-10 A. Kodre	IV-O-37 J. Nilsson	II-O-15 K. Klementiev
	Anisotropies and Magnetic coupling in MnFe2O4@CoFe2O4 core@shell nanoparticles	EXAFS study of mercury ligand environment in mycorrhizal plant roots	Dynamics of supported palladium nanoparticles during methane oxidation studied by in situ XAFS	High performance emission spectrometer at Balder/MAX IV beamline
12:10		VIII-O-11 C. Streeck	IV-O-38 C. Prestipino	II-O-16 T. Regier
		Detection of protein attachment at functionalized solid-liquid interfaces by X-ray absorption spectrometry of carbon and nitrogen	In situ EXAFS investigation of Ce1-xFexO2-x/2 solid solution for oxygen buffer application	An ambient pressure capable soft x-ray microprobe at the Canadian Light Source
12:30	Lunch break			12:30
13:40	VIII-PL-09 Hugh Harris X-ray probes for heavy elements in health and disease	B. Bunker		13:40
14:20	Presentation of XAFS17 in Krakow/Poland W. Kwiatek			14:20
14:40	Closing remarks New president of IXAS; J.-D. Grunwaldt, XAFS16 chair			14:40
15:00	ANKA tour			15:00
18:00	Sino-German Workshop on Catalysis and Membranes (Official end of workshop: Saturday, 29.08.2015 17:15)			18:00

Topic color code

General

II. New sources and new instrumentation

IV. Chemistry, catalysis, operando and time-resolved studies

VI. Materials Science

VIII. Soft Matter and biology

Travel and Directions

Karlsruhe is easily accessible from a number of airports, rail connections and highways:

Airports

- Stuttgart
- Frankfurt
- Karlsruhe / Baden-Baden
- Strasbourg airport in France

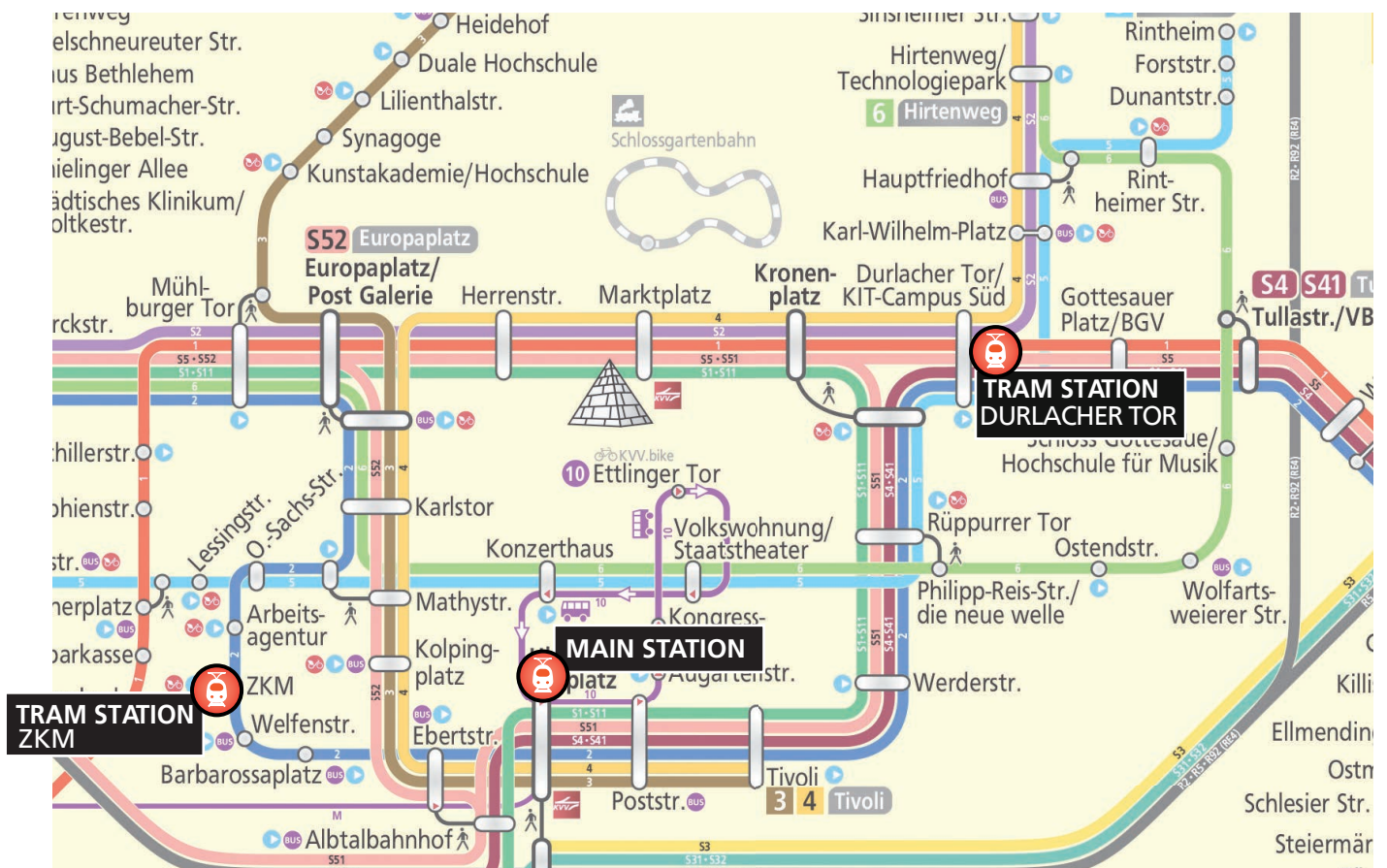
Rail connections

- From Berlin, Hamburg, Frankfurt, Stuttgart, Basel (ICE), Paris (TGV)
- Tram lines from Karlsruhe Main Train Station: 2, S41, S4, 4 (to tram station „Durlacher Tor“)



Conference Venue

- KIT Campus South | Karlsruhe Institute of Technology, Kaiserstraße 12, 76131 Karlsruhe
 - **Building 30.95: Audimax (A/B)**, Straße am Forum 1, 76131 Karlsruhe
 - **Building 30.41: Chemie HS I / Criegee**, Fritz-Haber-Weg 2-6, 76131 Karlsruhe
 - **Building 30.46: Neue Chemie**, Engesserstraße 15, 76131 Karlsruhe
 - **Building 01.13: MENSA**, Straße am Forum 4, 76131 Karlsruhe
- Oral Presentations
(see map on page 15-17)
- KIT Campus North | Karlsruhe Institute of Technology, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen
 - **Building 348: ANKA** - Synchrotron Radiation Facility, KIT Campus North
- **ZKM**: Lorenzstraße 19, 76135 Karlsruhe (tram station „ZKM“)

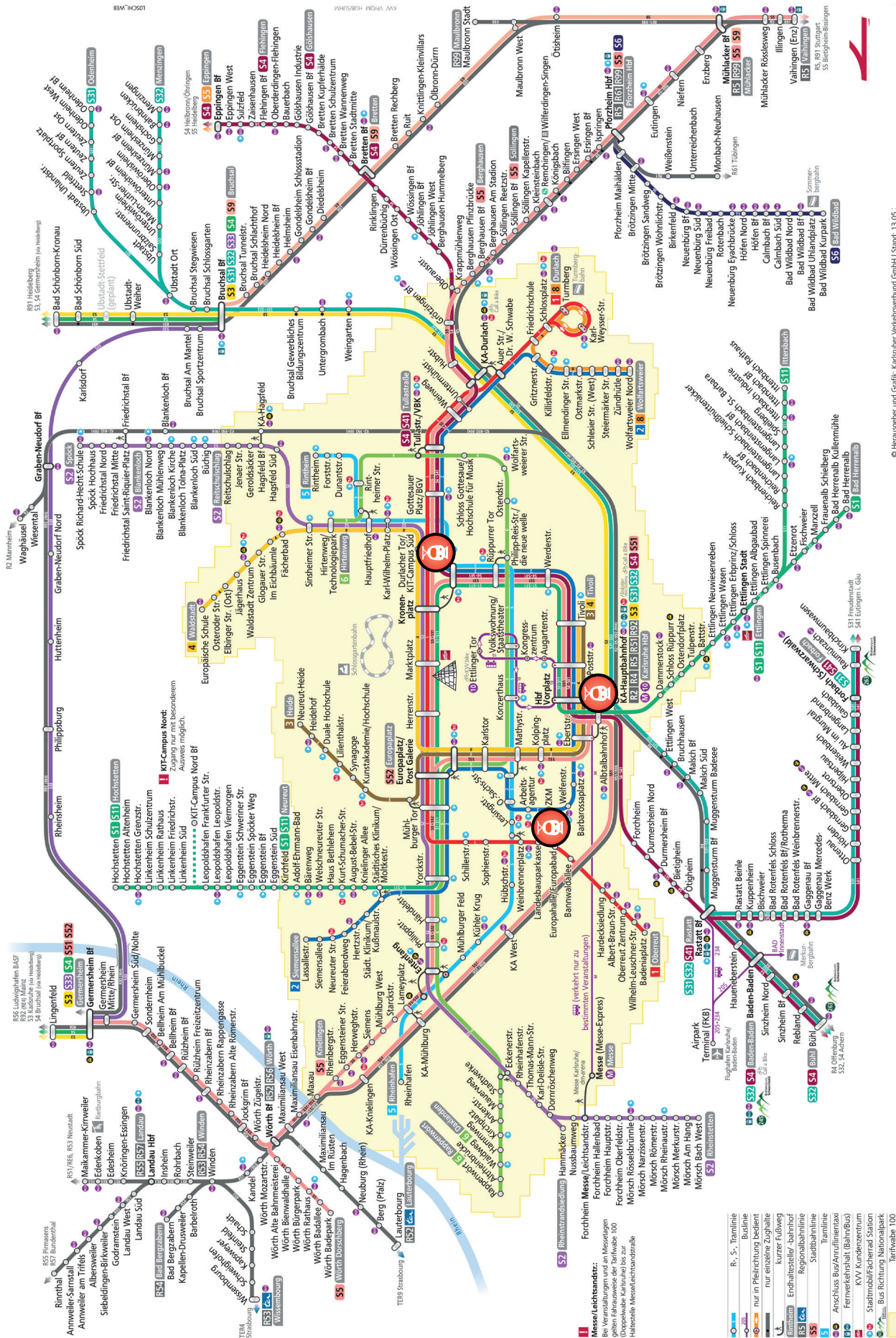


Public Transport (KVV plan)

Gültig ab 08. Juni 2015



Linienetzplan

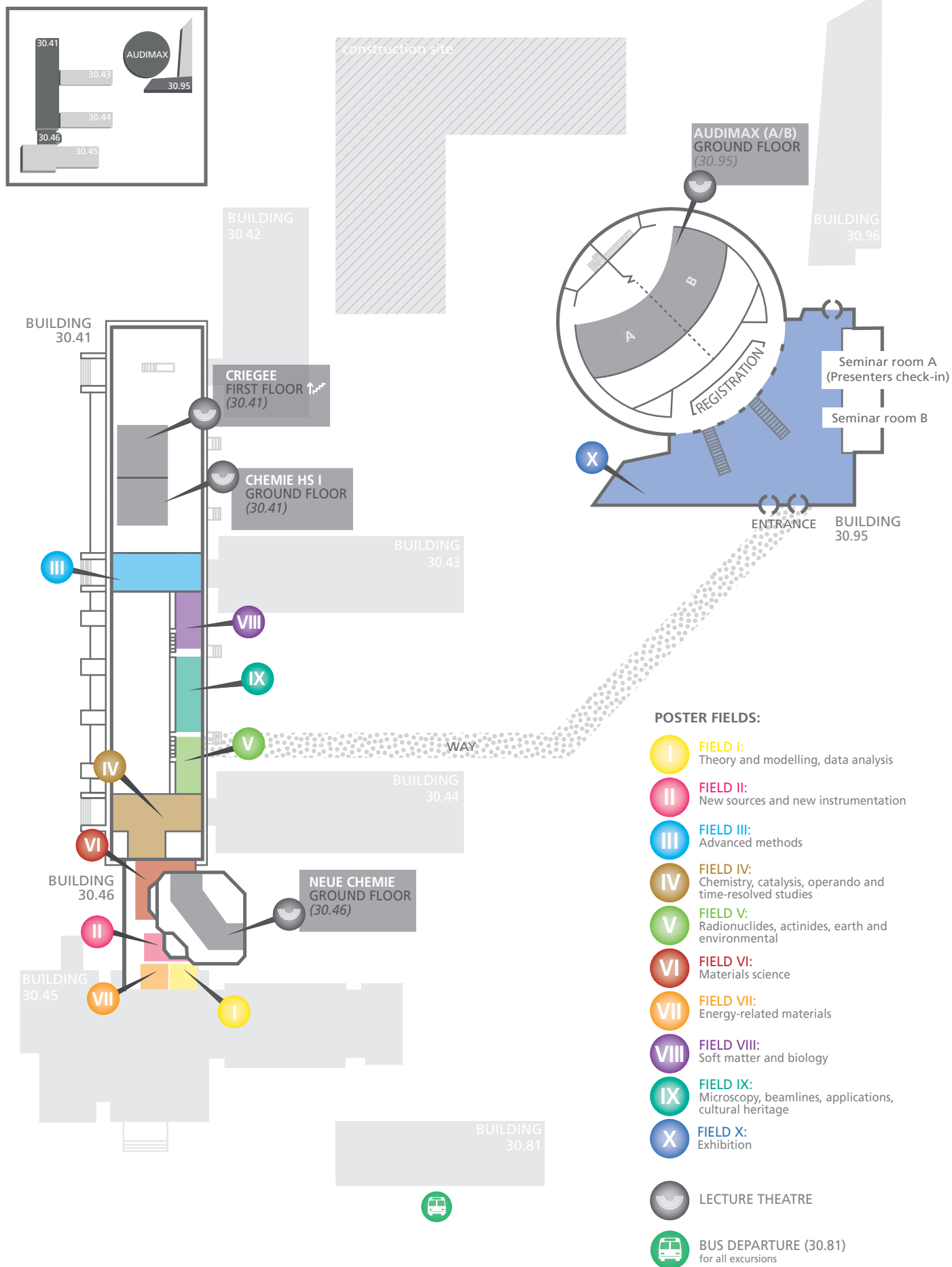


The map displays the KIT Campus Süd with various buildings and streets. Key locations include:

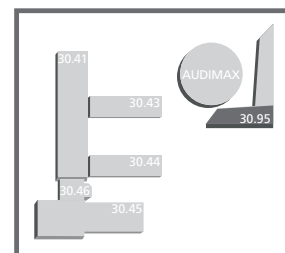
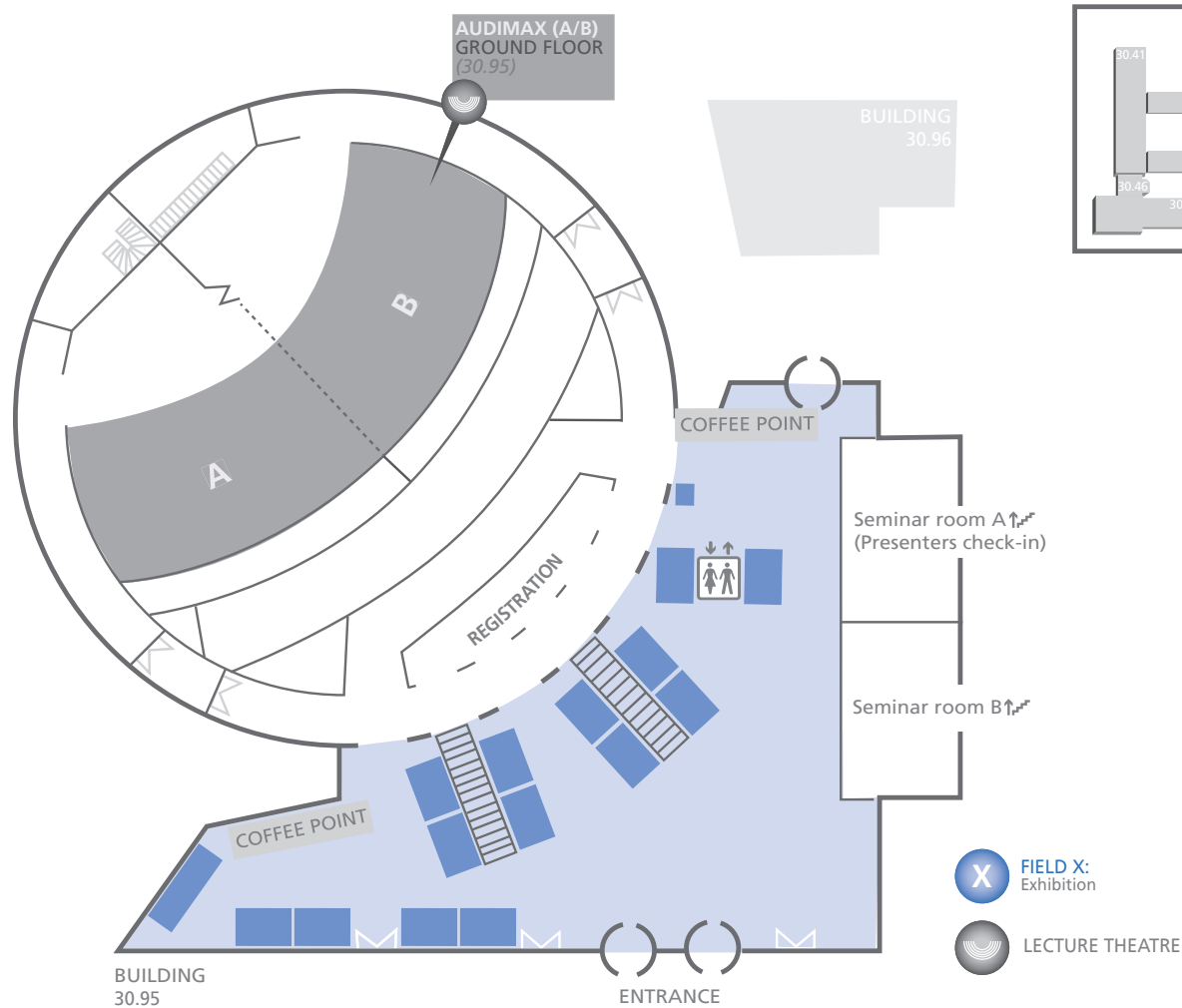
- Waldparkplatz** (Parking) at the top right.
- TRAM STATION** at the top left.
- LECTURE THEATRE** (indicated by a semi-circle icon) near the center.
- BUS DEPARTURE** for all excursions (30.81) at the bottom center.
- TRAM STATION DURLACHER TOR** at the bottom.
- Buildings and Floors:**
 - CRIGEE FIRST FLOOR** (30.41)
 - CHEMIE HS I GROUND FLOOR** (30.41)
 - AUDIMAX (A/B) GROUND FLOOR** (30.95)
 - NEUE CHEMIE GROUND FLOOR** (30.46)
- Other Labels:** Canteen, KIT-Shuttle, Studentenzentrum, Engesserstraße, Engler-Bunke-Ring, Adenauer-Ring, Am Fasanengarten, Richard-Willstätter-Allee, Hagsfelder Allee, Leimannstraße, Wolfgang-Gr., Irene-Rosenberg-Straße, Engelbert-Arnold-Straße, Otto-Ammann-Platz, R.-Baumeister-Platz, Durlacher Allee, Waldhornstraße, Fritz-Ehrlich-Straße, Berliner Platz, Ehrenhof, Wilhelm-Nusselt-Weg, Ernst-Gaber-Str., Haupteneinfahrt, Einfahrt.



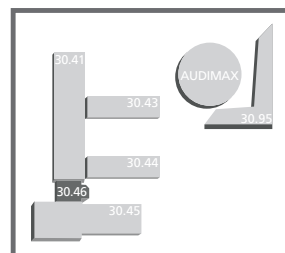
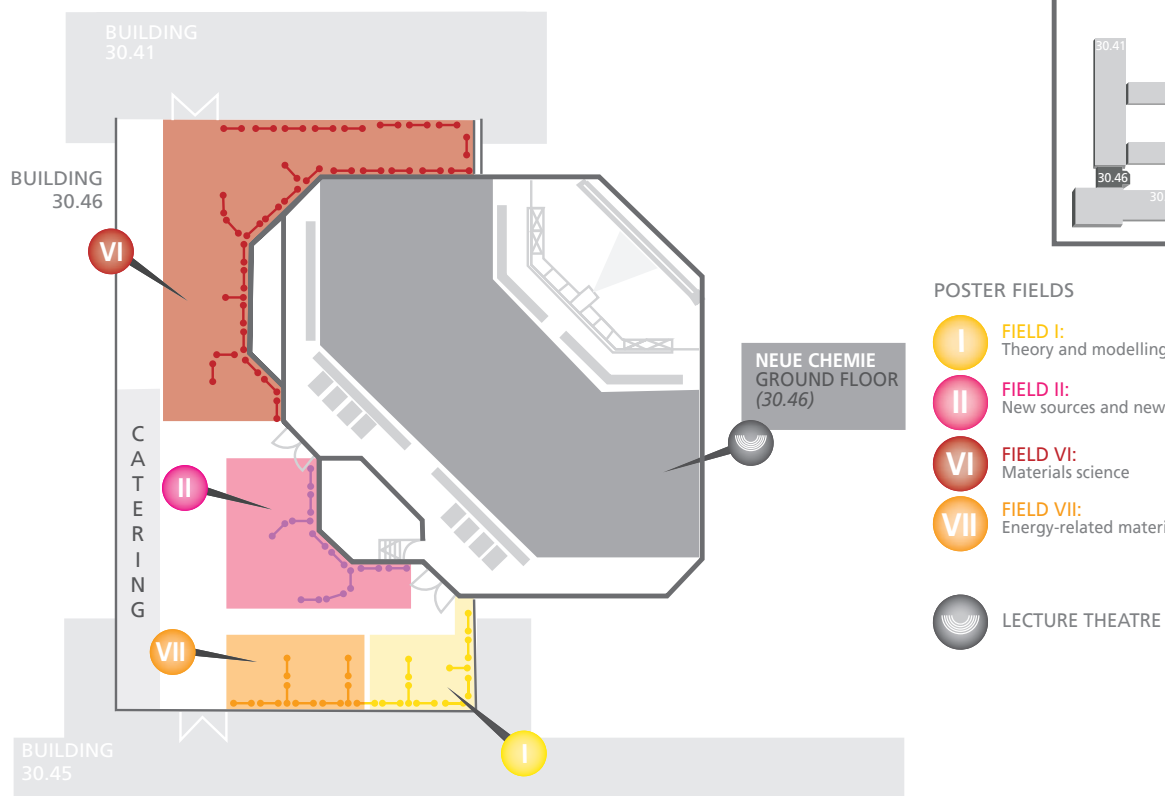
Conference Venue



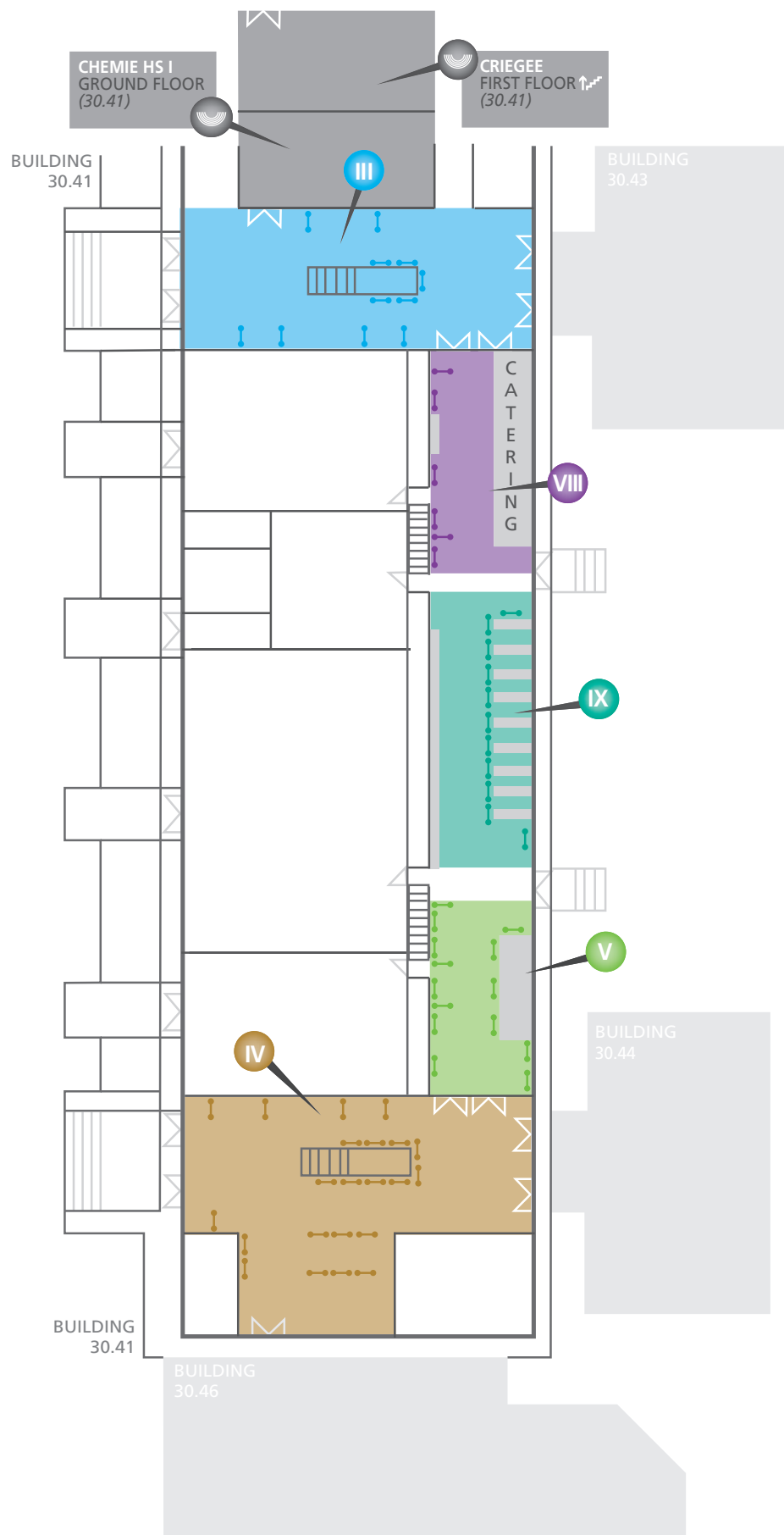
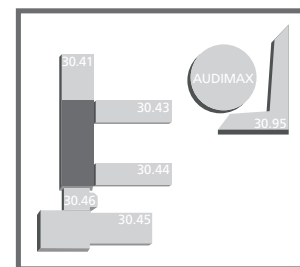
Lecture Halls | Exhibition: Audimax



Lecture Halls | Poster Sessions: Building 30.46



Lecture Halls | Poster Sessions: Building 30.41



POSTER FIELDS:

-  **FIELD III:**
Advanced methods
-  **FIELD IV:**
Chemistry, catalysis, operando and time-resolved studies
-  **FIELD V:**
Radionuclides, actinides, earth and environmental
-  **FIELD VIII:**
Soft matter and biology
-  **FIELD IX:**
Microscopy, beamlines, applications, cultural heritage
-  **LECTURE THEATRE**

Social Events

Welcome Party

Sunday, August 23, 18:00–20:00 h, Audimax (KIT Campus South)

Take the opportunity to get to know the other participants better and enjoy delicious fire-baked Flammkuchen (flaming cakes) at the Audimax at Campus South.

Welcome Party admission is included in your conference registration. Voucher will be handed over at the registration desk.



Excursions

Wednesday, August 26, 14:00–19:10 h (after lunch)

Wednesday afternoon is reserved for optional excursions. Three different guided tours are proposed. The number of participants may be restricted. Tours will be booked following the rule “first registered, first served”.

The three options are as follows:

- A walking tour of Heidelberg’s Old Town,
- A wine tasting tour in Affental Valley located near Baden-Baden,
- A visiting tour of the medieval Maulbronn Monastery (Unesco World Heritage Site).

The detailed information given below is provided by Karlsruhe Tourismus in charge of the guided tour organization.

Walking tour of Heidelberg’s Old Town

Enchanting alleys and squares, small gardens that pop up unexpectedly, museums and galleries: Heidelberg’s Old Town has many facets. So that you do not miss any of it, we offer guided walks around the Old Town. Our tours will breathe life into the city’s past, adding rich detail to the contours of today’s city.

Whether it is the Heiliggeistkirche (Church of the Holy Spirit), the Jesuit district, Germany’s oldest Univ. with its Studentenkärzer (Students’ Prison), or the other sight-seeing attractions: every place of interest in the Old Town has a unique ambiance and history well worth immersing yourself in for a few minutes. The tour also passes along the Hauptstrasse (Main Street), one of the largest pedestrian zones in Europe.

Many detours into the alleyways of the Old Town confirm once again the truth of the sentence which says “only truly learn about the countryside by taking the back roads.”

The excursion takes around 6 hours and includes:

- Bus trip from Karlsruhe (Meeting Point: in front of Building 30.81) to Karlsruhe,
- Guest Guide (language: English),
- 3 hours Walking Tour Old Town, (language: English), Funicular Railway and entrance to castle,
- Free open time (ca. 1 hour),

Price: € 38 per pers. – 50 pers. / bus.



A Wine tasting tour in Affental valley

Affental is located in the district of Baden, Germany's southern most wine-growing region. Here amid the warm climate of the Rhine Vally at the foot of the Black Forest, spring begins early. Warm granite-weathered soil on the steep Black forest precipices and strong loess terrain on the soft foothills are best suited for the cultivation of Pinot Noir and Rieslings.

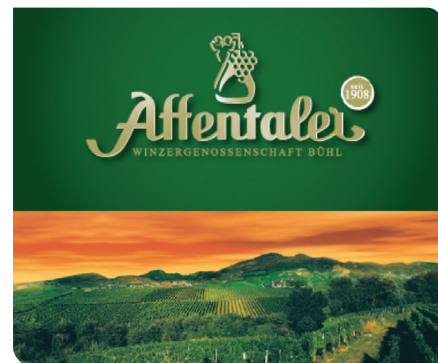
The excursion takes around 5 hours and includes:

- Bus trip from and to Karlsruhe (Meeting Point: in front of Bld. 30.81),
- Guest Guide (language: English),
- Wine cellar tour (45 min),
- 6 wine type-tastings,

Price: € 37 per pers. - 50 pers. / bus.

6 wine type-tastings:

- Rivaner QbA dry "Primus",
- Riesling QbA "Affentaler Edition",
- Grauer Burgunder Spätlese (Late Harvest) "Primus",
- Pinot Noir Rosé Cabinet "Affentaler Edition",
- Pinot Noir red wine QbA "Monkey bottle",
- Pinot Noir QbA dry red wine "Buddle".



Visit of the Maulbronn Monastery (Unesco World Heritage Site)

Maulbronn Monastery (Kloster Maulbronn) is one of Europe's most complete and best preserved Medieval monastery complexes. It combines a multitude of architectural styles, from Romanesque to late Gothic, in one place – creating a unique atmosphere.

The excursion takes around 4 hours and includes:

- Bus trip from Karlsruhe (Meeting Point: in front of Building 30.81) to Karlsruhe,
- Guest Guide (language: English),
- Monastery tour, 1 hour,
- Opportunity visiting restaurant "Klosterschmiede",
- Opportunity footpath to lake "Tiefensee" (10 min).

Price: € 34 per pers. – 50 pers. / bus.



ZKM (Center for Art and Media) – Tour

Thursday, August 27, 18:00 – 19:00 h

By extending the original duties of a museum, the ZKM has become a cultural Institute unique throughout the world. It is a house for all media and genre, a house for both spatially-based arts, such as painting, photography and sculpture as well as time-based arts, such as film, video, media art, music, dance, theater, and performance. The tour through the ZKM lasts one hour, from 18:00–19:00 h and is included in the conference dinner.



Conference Dinner at ZKM (Center for Art and Media)

Thursday, August 27, 19:00 – 23:00 h

The experienced catering team of “Schloss Eberstein Gourmet Catering” with top chef Bernd Werner is caring about the success of the conference dinner. Hence, a catering with fantastic taste is guaranteed.

Schloss Eberstein Gourmet Catering offers creative cuisine, first-class products, excellent service and a realization at highest level.



Travel

ZKM

Lorenzstraße 19

76135 Karlsruhe

Travel by tram

- Tram line 2 from Karlsruhe “Durlacher Tor” via “Main Train Station” in the direction of “ZKM – Siemensallee” to **tram station ZKM**

ANKA Guided Tour

Friday, August 28, 15:00–17:30 h

Bus trip to KIT Campus North, Meeting Point: in front of Building 30.81 at 15:00 h. Return at about 17:30 h.

Take the opportunity to visit the Synchrotron Radiation Facility ANKA at KIT Campus North. The guided tour consists of an introductory presentation of the main methods, experimental stations and research fields at ANKA. After that, divided groups pass various stations like beamlines or laboratories where ANKA scientists present instrumentations and their applications.

