

**XAFS16**

# **Report of Contributions**

Contribution ID: 1

Type: **not specified**

# **X-ray emission spectroscopic studies of biological catalysis**

*Monday, August 24, 2015 9:30 AM (30 minutes)*

**Presenter:** Mrs DE BEER, Serena

**Session Classification:** III: Advanced Methods

Contribution ID: 5

Type: **not specified**

## Dynamic structural disorder and reactivity in supported metal nanocatalysts

*Monday, August 24, 2015 11:00 AM (20 minutes)***Presenter:** VILA, F.D.**Session Classification:** I: Theory and Modelling, Data analysis

Contribution ID: 6

Type: **not specified**

## **Advances in the theory and calculation of many-body effects in x-ray spectra**

*Monday, August 24, 2015 10:30 AM (30 minutes)*

**Presenter:** KAS, J.J.

**Session Classification:** I: Theory and Modelling, Data analysis

Contribution ID: 8

Type: **not specified**

## Efficient Bethe-Salpeter equation calculations of x-ray spectra of large systems

*Monday, August 24, 2015 11:20 AM (20 minutes)***Presenter:** GILMORE, K.**Session Classification:** I: Theory and Modelling, Data analysis

Contribution ID: 9

Type: **not specified**

## **Coordination environment of Hg(II) bound to E. coli in the presence and absence of organic ligands: influence of metabolic activity**

*Monday, August 24, 2015 10:40 AM (20 minutes)*

**Presenter:** Mrs THOMAS, Sara (Department of Civil and Environmental Engineering, Northwestern University, Evanston, IL US)

**Session Classification:** V: Radionuclides, actinides, earth and environmental

Contribution ID: 10

Type: **not specified**

## **An X-ray absorption spectroscopy study of Cd binding onto a halophilic archaeon**

*Monday, August 24, 2015 11:00 AM (20 minutes)*

**Author:** Mr SHOWALTER, A.R.

**Presenter:** Mr SHOWALTER, A.R.

**Session Classification:** V: Radionuclides, actinides, earth and environmental

Contribution ID: 11

Type: **not specified**

## Absorption and Mobility of Cr and Zn in Soil in the Vicinity of Jordan River

*Monday, August 24, 2015 11:20 AM (20 minutes)*

**Author:** Mr HARFOUCHE, Messaoud (Synchrotron-light for Experimental Science and Applications in the Middle East, Jordan)

**Presenter:** Mr HARFOUCHE, Messaoud (Synchrotron-light for Experimental Science and Applications in the Middle East, Jordan)

**Session Classification:** V: Radionuclides, actinides, earth and environmental



Contribution ID: 12

Type: **not specified**

## **Zn K-edge XAFS for the study of river material reactivity towards metals**

*Monday, August 24, 2015 11:40 AM (20 minutes)*

**Author:** Mr LE MEUR, Mathieu (Laboratoire Interdisciplinaire des Environnements Continentaux, CNRS Université de Lorraine, 15 avenue du Charmois, Vandœuvre lès Nancy, France)

**Presenter:** Mr LE MEUR, Mathieu (Laboratoire Interdisciplinaire des Environnements Continentaux, CNRS Université de Lorraine, 15 avenue du Charmois, Vandœuvre lès Nancy, France)

**Session Classification:** V: Radionuclides, actinides, earth and environmental

Contribution ID: 13

Type: **not specified**

## Origin of giant electrostriction in Gd doped ceria revealed by differential QEXAFS

*Monday, August 24, 2015 10:40 AM (20 minutes)*

**Author:** Mr LI, Yuanyuan (Department of Physics, Yeshiva University, New York, New York, United States)

**Presenter:** Mr LI, Yuanyuan (Department of Physics, Yeshiva University, New York, New York, United States)

**Session Classification:** IV: Chemistry, catalysis, operando and time-resolved studies

Contribution ID: 14

Type: **not specified**

## Quick XAFS system with millisecond time resolution

*Monday, August 24, 2015 11:00 AM (20 minutes)*

**Author:** Mr URUGA, Tomoya (Japan Synchrotron Radiation Research Institute, SPring-8, Japan; The University of Electro-Communications, Innovation Research Center for Fuel Cells, Japan)

**Presenter:** Mr URUGA, Tomoya (Japan Synchrotron Radiation Research Institute, SPring-8, Japan; The University of Electro-Communications, Innovation Research Center for Fuel Cells, Japan)

**Session Classification:** IV: Chemistry, catalysis, operando and time-resolved studies

Contribution ID: 15

Type: **not specified**

## ROCK: the Quick-EXAFS beamline at SOLEIL

*Monday, August 24, 2015 11:20 AM (20 minutes)*

**Presenter:** Mrs BARTHE, Laurent (ynchrotron SOLEIL, Gif-sur-Yvette, France)

**Session Classification:** IV: Chemistry, catalysis, operando and time-resolved studies

Contribution ID: 16

Type: **not specified**

## Nucleation and Growth Kinetics of Multinary Nanocrystals by Quick Extended X-ray Absorption Fine Structure

*Monday, August 24, 2015 11:40 AM (20 minutes)*

**Presenter:** Mr JUST, Justus (Bergische Universität Wuppertal, Wuppertal, Germany; Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany)

**Session Classification:** IV: Chemistry, catalysis, operando and time-resolved studies

Contribution ID: 17

Type: **not specified**

## State-dependent fluorescence through the Coulomb exchange

*Monday, August 24, 2015 10:40 AM (20 minutes)***Presenter:** MIEDEMA, Piter S. (FG-ISRR, Helmholtz-Zentrum Berlin, Germany)**Session Classification:** III: Advanced Methods

Contribution ID: 19

Type: **not specified**

## Orbital mixing and multiplet effects in the K absorption pre-edges of TiO<sub>2</sub> and Mn<sub>2</sub>O<sub>3</sub>

*Monday, August 24, 2015 11:20 AM (20 minutes)*

**Presenter:** Mr GLATZEL, Pieter (European Synchrotron Radiation Facility, Grenoble, France)

**Session Classification:** III: Advanced Methods

Contribution ID: 20

Type: **not specified**

## Non-resonant X-ray Raman scattering spectroscopy

*Monday, August 24, 2015 11:40 AM (30 minutes)***Author:** Mr HUOTARI, Simo (Department of Physics, University of Helsinki, Finland)**Presenter:** Mr HUOTARI, Simo (Department of Physics, University of Helsinki, Finland)**Session Classification:** III: Advanced Methods



Contribution ID: 23

Type: **not specified**

## **Extracting Electronic Structure Information from 1s2p RIXS and L-edge XAS of Transition Metal Complexes**

*Monday, August 24, 2015 11:00 AM (20 minutes)***Presenter:** KROLL, T.**Session Classification:** III: Advanced Methods

Contribution ID: 24

Type: **not specified**

## **FEFF85EXAFS: open source theoretical standards for EXAFS analysis**

*Monday, August 24, 2015 11:40 AM (20 minutes)*

**Presenter:** RAVEL, B.

**Session Classification:** I: Theory and Modelling, Data analysis

Contribution ID: 25

Type: **not specified**

## **A toolbox for the strong-field representation of charge transfer multiplets of transition metal compounds**

*Monday, August 24, 2015 1:30 PM (20 minutes)*

**Author:** DELGADO-JAIME, M.U.

**Presenter:** DELGADO-JAIME, M.U.

**Session Classification:** I: Theory and Modelling, Data analysis

Contribution ID: 26

Type: **not specified**

## **EXAFS analysis using the new Graphical User Interface of the GNXAS suite of programs**

*Monday, August 24, 2015 1:50 PM (20 minutes)***Presenter:** HATADA, K.**Session Classification:** I: Theory and Modelling, Data analysis

Contribution ID: 27

Type: **not specified**

**Disappearance of correlations in the atom motion  
upon hydrogen intercalation into ReO<sub>3</sub> lattice:  
in-situ EXAFS study, deciphered by a novel reverse  
Monte Carlo/evolutionary algorithm approach**

*Monday, August 24, 2015 2:10 PM (20 minutes)*

**Presenter:** TIMOSHENKO, J.

**Session Classification:** I: Theory and Modelling, Data analysis

Contribution ID: 28

Type: **not specified**

## **High-Flux EXAFS Beamline P64 at PETRAIII**

*Monday, August 24, 2015 5:00 PM (20 minutes)*

**Presenter:** CALIEBE, W.

**Session Classification:** II. New sources and new instrumentation

Contribution ID: 29

Type: **not specified**

## **The new QEXAFS monochromator, detection and data acquisition system at the SuperXAS beamline (SLS) for EXAFS spectroscopy with 15 ms time resolution**

*Monday, August 24, 2015 5:20 PM (20 minutes)*

**Presenter:** MÜLLER, O.

**Session Classification:** II. New sources and new instrumentation

Contribution ID: 30

Type: **not specified**

## **Progress in XANES ab initio calculations of complex metalloenzymes with two metal centers**

*Monday, August 24, 2015 2:20 PM (20 minutes)*

**Presenter:** CHU, W.S.

**Session Classification:** V: Radionuclides, actinides, earth and environmental



Contribution ID: 31

Type: **not specified**

## **Metal-hydride intermediates in FeFe and NiFe hydrogenase enzymes detected and characterized by XAS/XES and DFT**

*Monday, August 24, 2015 2:00 PM (20 minutes)***Presenter:** KOSITZKI, R.**Session Classification:** V: Radionuclides, actinides, earth and environmental

Contribution ID: 32

Type: **not specified**

## **Insights into the electronic structure of iron atoms in FeMo cofactor of nitrogenase and related models**

*Monday, August 24, 2015 1:40 PM (20 minutes)***Presenter:** KOWALSKA, J.**Session Classification:** V: Radionuclides, actinides, earth and environmental

Contribution ID: 33

Type: **not specified**

## **Zn(II)/Cu(II) cross-coordination to Ab peptides can modulate the peptide aggregation propensity. A XAS structural study**

*Monday, August 24, 2015 1:20 PM (20 minutes)*

**Presenter:** DE SANTIS, E.

**Session Classification:** V: Radionuclides, actinides, earth and environmental

Contribution ID: 34

Type: **not specified**

## Characterization of surface contaminants of medical devices

*Monday, August 24, 2015 2:40 PM (20 minutes)***Presenter:** POLLAKOWSKI, B.**Session Classification:** V: Radionuclides, actinides, earth and environmental

Contribution ID: 35

Type: **not specified**

## **Local environment and electronic structure of active sites in Cu-SSZ-13 deNO<sub>x</sub> catalyst under reaction conditions**

*Monday, August 24, 2015 2:00 PM (20 minutes)*

**Presenter:** LAMBERTI, C.

**Session Classification:** IV: Chemistry, catalysis, operando and time-resolved studies

Contribution ID: 36

Type: **not specified**

## **Confinement effects of carbon nanotubes on catalysis**

*Monday, August 24, 2015 2:20 PM (20 minutes)***Presenter:** ZHANG, F.**Session Classification:** IV: Chemistry, catalysis, operando and time-resolved studies

Contribution ID: 37

Type: **not specified**

## **Mechanochemical preparation and local structural analysis of Pd-LaFeO<sub>3</sub> solid solutions by Pd K- and L<sub>3</sub>-edge X-ray absorption spectroscopy**

*Monday, August 24, 2015 1:40 PM (20 minutes)*

**Presenter:** UCHIYAMA, T.

**Session Classification:** IV: Chemistry, catalysis, operando and time-resolved studies

Contribution ID: 39

Type: **not specified**

**Geometric and electronic structure of Au on  
Au/CeO<sub>2</sub> catalysts during the CO oxidation:  
Deactivation by reaction induced particle growth**

*Monday, August 24, 2015 1:20 PM (20 minutes)*

**Presenter:** ABDEL-MAGEED, A.M.

**Session Classification:** IV: Chemistry, catalysis, operando and time-resolved studies



Contribution ID: 40

Type: **not specified**

## **Operando structure-activity correlations in applied catalytic systems: Oscillatory CO oxidation in exhaust gas catalysts**

*Monday, August 24, 2015 2:40 PM (20 minutes)*

**Presenter:** GÄNZLER, A.

**Session Classification:** IV: Chemistry, catalysis, operando and time-resolved studies

Contribution ID: 41

Type: **not specified**

## **Efficient multicore parallelization of the finite difference method for x-ray absorption spectroscopy in the FDMNES code**

*Monday, August 24, 2015 2:30 PM (20 minutes)***Presenter:** GUDA, A.A.**Session Classification:** I: Theory and Modelling, Data analysis

Contribution ID: 42

Type: **not specified**

## **X-ray absorption spectra of graphene and graphene oxide by Full Potential Multiple Scattering calculations with self-consistent potential**

*Monday, August 24, 2015 2:50 PM (20 minutes)***Presenter:** JUNQUIG, X.**Session Classification:** I: Theory and Modelling, Data analysis

Contribution ID: 43

Type: **not specified**

## **Novel Structural Chemistry –and More –from Actinide XAFS**

**Presenter:** CONRADSON, S.

Contribution ID: 44

Type: **not specified**

## **High energy resolution XANES as a tool for electronic and geometric structural investigations of actinide materials**

**Presenter:** VITOVA, T.

Contribution ID: 45

Type: **not specified**

**Biological and abiotic factors affecting the  
solid-phase speciation of U(IV) following reduction  
of aqueous U(VI)**

**Presenter:** BOYANOV, M.I.

Contribution ID: 46

Type: **not specified**

**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**

**Presenter:** SAMSON, V.A.

Contribution ID: 47

Type: **not specified**

## **Speciation of neptunium during sorption and diffusion in natural clay**

**Presenter:** REICH, T.



Contribution ID: 48

Type: **not specified**

## **Local environment and electronic structure of active sites in Cu-SSZ-13 deNO<sub>x</sub> catalyst under reaction conditions**

**Presenter:** LAMBERTI, C.

Contribution ID: 49

Type: **not specified**

## **In-situ 2p3d resonant x-ray emission spectroscopy of Co/CNT Fischer-Tropsch catalysts**

**Presenter:** LIU, B.

Contribution ID: 50

Type: **not specified**

**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**

**Presenter:** KOPELINT, R.

Contribution ID: 51

Type: **not specified**

## **XAFS Investigations of MoO<sub>x</sub>/Fe<sub>2</sub>O<sub>3</sub> based systems**

**Presenter:** WELLS, P.P.

Contribution ID: 52

Type: **not specified**

## **Investigation of preferential CO oxidation over Co<sub>3</sub>O<sub>4</sub> and CeO<sub>2</sub>-Co<sub>3</sub>O<sub>4</sub> by operando X-ray absorption spectroscopy**

**Presenter:** LUKASHUK, L.

Contribution ID: 53

Type: **not specified**

## **Tracking of the changes during nucleation and growth of nanoparticles in solution –MCR-ALS analysis of time-resolved XANES data**

*Monday, August 24, 2015 1:30 PM (20 minutes)***Presenter:** STANIUK, M.**Session Classification:** VI: Material Science

Contribution ID: 54

Type: **not specified**

## **Interfacial water on nanodiamonds in colloidal dispersions probed by transmission X-ray absorption spectroscopy**

*Monday, August 24, 2015 1:50 PM (20 minutes)***Presenter:** PETIT, T.**Session Classification:** VI: Material Science

Contribution ID: 55

Type: **not specified**

## **In situ XAS uncovering the mechanisms of thermal stabilization of polymer-clay nanocomposites**

*Monday, August 24, 2015 2:10 PM (20 minutes)***Presenter:** CARVALHO, H.W.P.**Session Classification:** VI: Material Science



Contribution ID: 56

Type: **not specified**

## **Characterizing the structural properties of the NPs formed by ion implantation in LPCVD and PECVD Si<sub>3</sub>N<sub>4</sub> using XAS**

*Monday, August 24, 2015 2:30 PM (20 minutes)***Presenter:** MIRZAEI, S.**Session Classification:** VI: Material Science

Contribution ID: 57

Type: **not specified**

## **Advanced ultralow-k organosilicate glasses: NEXAFS study**

*Monday, August 24, 2015 2:50 PM (20 minutes)***Presenter:** KONASHUK, A.**Session Classification:** VI: Material Science

Contribution ID: 58

Type: **not specified**

## **Upgraded X-ray Spectroscopy Microprobe Beamline 13-ID-E of the Advanced Photon Source**

*Monday, August 24, 2015 3:50 PM (30 minutes)*

**Presenter:** NEWVILLE, M.

**Session Classification:** II. New sources and new instrumentation

Contribution ID: 59

Type: **not specified**

## **X-ray Absorption Spectroscopy under Extremes**

*Monday, August 24, 2015 4:20 PM (20 minutes)***Presenter:** MATHON, O.**Session Classification:** II. New sources and new instrumentation

Contribution ID: 60

Type: **not specified**

## Quick XAFS system with millisecond time resolution

*Monday, August 24, 2015 4:40 PM (20 minutes)***Presenter:** URUGA, T.**Session Classification:** II. New sources and new instrumentation

Contribution ID: **61**

Type: **not specified**

## **High-Flux EXAFS Beamline P64 at PETRAIII**

**Presenter:** CALIEBE, W.

Contribution ID: 62

Type: **not specified**

## **The new QEXAFS monochromator, detection and data acquisition system at the SuperXAS beamline (SLS) for EXAFS spectroscopy with 15 ms time resolution**

**Presenter:** MÜLLER, O.

Contribution ID: 63

Type: **not specified**

## **Progress in XANES ab initio calculations of complex metalloenzymes with two metal centers**

*Monday, August 24, 2015 3:50 PM (30 minutes)***Presenter:** CHU, W.S.**Session Classification:** VIII: Soft Matter and biology



Contribution ID: 64

Type: **not specified**

## **Metal-hydride intermediates in FeFe and NiFe hydrogenase enzymes detected and characterized by XAS/XES and DFT**

*Monday, August 24, 2015 4:20 PM (20 minutes)***Presenter:** KOSITZKI, R.**Session Classification:** VIII: Soft Matter and biology

Contribution ID: 65

Type: **not specified**

## **Insights into the electronic structure of iron atoms in FeMo cofactor of nitrogenase and related models**

*Monday, August 24, 2015 4:40 PM (20 minutes)***Presenter:** KOWALSKA, J.**Session Classification:** VIII: Soft Matter and biology

Contribution ID: 66

Type: **not specified**

## **Zn(II)/Cu(II) cross-coordination to Ab peptides can modulate the peptide aggregation propensity. A XAS structural study**

*Monday, August 24, 2015 5:00 PM (20 minutes)***Presenter:** DE SANTIS, E.**Session Classification:** VIII: Soft Matter and biology

Contribution ID: 67

Type: **not specified**

## Characterization of surface contaminants of medical devices

*Monday, August 24, 2015 5:20 PM (20 minutes)***Presenter:** POLLAKOWSKI, B.**Session Classification:** VIII: Soft Matter and biology

Contribution ID: 68

Type: **not specified**

## **Precise observation of structural change of Pd nanoparticles during surface adsorption and catalytic reaction**

*Monday, August 24, 2015 4:00 PM (20 minutes)***Presenter:** MATSUMURA, D.**Session Classification:** IV: Chemistry, catalysis, operando and time-resolved studies

Contribution ID: 69

Type: **not specified**

## **Confinement effects of carbon nanotubes on catalysis**

*Monday, August 24, 2015 4:20 PM (20 minutes)***Presenter:** ZHANG, F.**Session Classification:** IV: Chemistry, catalysis, operando and time-resolved studies

Contribution ID: 70

Type: **not specified**

## **Mechanochemical preparation and local structural analysis of Pd-LaFeO<sub>3</sub> solid solutions by Pd K- and L<sub>3</sub>-edge X-ray absorption spectroscopy**

*Monday, August 24, 2015 4:40 PM (20 minutes)*

**Presenter:** UCHIYAMA, T.

**Session Classification:** IV: Chemistry, catalysis, operando and time-resolved studies

Contribution ID: 71

Type: **not specified**

**Geometric and electronic structure of Au on  
Au/CeO<sub>2</sub> catalysts during the CO oxidation:  
Deactivation by reaction induced particle growth**

*Monday, August 24, 2015 5:00 PM (20 minutes)*

**Presenter:** ABDEL-MAGEED, A.M.

**Session Classification:** IV: Chemistry, catalysis, operando and time-resolved studies



Contribution ID: 72

Type: **not specified**

## **Operando structure-activity correlations in applied catalytic systems: Oscillatory CO oxidation in exhaust gas catalysts**

*Monday, August 24, 2015 5:20 PM (20 minutes)*

**Presenter:** GÄNZLER, A.

**Session Classification:** IV: Chemistry, catalysis, operando and time-resolved studies

Contribution ID: 73

Type: **not specified**

## **Negative thermal expansion of ScF<sub>3</sub>: an EXAFS study at the Scandium K-edge from 10 K up to 1100 K**

*Monday, August 24, 2015 3:50 PM (30 minutes)***Presenter:** ALI, S.**Session Classification:** VI: Material Science

Contribution ID: 74

Type: **not specified**

## Identification of carbon bonds in graphene oxide using soft x-ray reflectometry

*Monday, August 24, 2015 4:20 PM (20 minutes)***Presenter:** WAHAB, H.**Session Classification:** VI: Material Science

Contribution ID: 75

Type: **not specified**

## **High-resolution x-ray absorption and emission spectroscopy study of Mn incorporation in Al<sub>x</sub>Ga<sub>1-x</sub>N hetero-structures**

*Monday, August 24, 2015 4:40 PM (20 minutes)***Presenter:** ROVEZZI, M.**Session Classification:** VI: Material Science

Contribution ID: 76

Type: **not specified**

## **Local atomic and electronic structure of ferroelectric materials: X-ray investigation and computer modeling**

*Monday, August 24, 2015 5:00 PM (20 minutes)***Presenter:** SUKHARINA, G.**Session Classification:** VI: Material Science

Contribution ID: 77

Type: **not specified**

## **Synthesis, characterization and modeling of i-Al<sub>65</sub>Cu<sub>23</sub>Fe<sub>12</sub> quasicrystals**

*Monday, August 24, 2015 5:20 PM (20 minutes)***Presenter:** POLOZHENTSEV, O.**Session Classification:** VI: Material Science

Contribution ID: 78

Type: **not specified**

## **Time-resolved x-ray absorption and emission spectroscopies to determine the structure of the catalytic active site**

**Presenter:** NACHTEGAAL, M.

Contribution ID: 79

Type: **not specified**

## **Yoneda-XAFS experiments with X-ray area detectors**

**Presenter:** GASSE, J.-C.



Contribution ID: 80

Type: **not specified**

## **Probing the magnetization dynamics of spin valve systems using x-detected ferromagnetic resonance**

*Tuesday, August 25, 2015 10:40 AM (20 minutes)*

**Presenter:** VAN DER LAAN, G.

**Session Classification:** III: Advanced Methods

Contribution ID: 81

Type: **not specified**

## **The quality of X-ray Absorption Fine Structure measurements by Transmission for dilute systems, using the Hybrid Technique**

*Tuesday, August 25, 2015 11:00 AM (20 minutes)***Presenter:** CHANTLER, C.T.**Session Classification:** III: Advanced Methods

Contribution ID: 82

Type: **not specified**

## **Time-resolved x-ray absorption and emission spectroscopies to determine the structure of the catalytic active site**

*Tuesday, August 25, 2015 11:20 AM (20 minutes)***Presenter:** NACHTEGAAL, M.**Session Classification:** III: Advanced Methods

Contribution ID: 83

Type: **not specified**

## Yoneda-XAFS experiments with X-ray area detectors

*Tuesday, August 25, 2015 11:40 AM (20 minutes)***Presenter:** GASSE, J.-C.**Session Classification:** III: Advanced Methods

Contribution ID: 84

Type: **not specified**

## Exploring the formation and structural diversity of Fe(III)-precipitates in aquatic systems using XAS

*Tuesday, August 25, 2015 10:30 AM (20 minutes)*

**Presenter:** VOEGELIN, A.

**Session Classification:** V: Radionuclides, actinides, earth and environmental

Contribution ID: 85

Type: **not specified**

## **Probing the 3d states of Fe in goethite using Al K-edge XANES spectroscopy**

*Tuesday, August 25, 2015 10:50 AM (20 minutes)***Presenter:** DUCHER, M.**Session Classification:** V: Radionuclides, actinides, earth and environmental

Contribution ID: 86

Type: **not specified**

## **Metal (Hydr)oxides for the removal of Cr(VI) from drinking**

*Tuesday, August 25, 2015 11:10 AM (20 minutes)*

**Presenter:** FANI, P.

**Session Classification:** V: Radionuclides, actinides, earth and environmental

Contribution ID: 87

Type: **not specified**

## **X-ray microspectroscopic investigations of heavy metal uptake by argillaceous rocks**

*Tuesday, August 25, 2015 11:30 AM (20 minutes)*

**Presenter:** DÄHN, R.

**Session Classification:** V: Radionuclides, actinides, earth and environmental



Contribution ID: 88

Type: **not specified**

## **Polarization dependent total reflection fluorescence XAFS and the control of metal structures on oxide surfaces**

*Tuesday, August 25, 2015 10:50 AM (20 minutes)*

**Presenter:** ASAKURA, K.

**Session Classification:** IV: Chemistry, catalysis, operando and time-resolved studies

Contribution ID: 89

Type: **not specified**

## **XAFS study of the local structure of iron on the (0001) surface of the topological insulator Bi<sub>2</sub>Se<sub>3</sub>**

*Tuesday, August 25, 2015 11:10 AM (20 minutes)*

**Presenter:** MEYERHEIM, H.L.

**Session Classification:** IV: Chemistry, catalysis, operando and time-resolved studies

Contribution ID: 90

Type: **not specified**

## Atomically precise semiconductor-graphene interfaces by Ge intercalation

*Tuesday, August 25, 2015 11:30 AM (20 minutes)***Presenter:** VERBITSKIY, N.I.**Session Classification:** IV: Chemistry, catalysis, operando and time-resolved studies

Contribution ID: 91

Type: **not specified**

## **The Role Of Ag and Sb Ions In The Resistive Switching Mechanism Of Conductive Bridging Random Access Memories**

*Tuesday, August 25, 2015 11:50 AM (20 minutes)***Presenter:** D'ACAPITO, F.**Session Classification:** IV: Chemistry, catalysis, operando and time-resolved studies

Contribution ID: 92

Type: **not specified**

## **Thermo-mechanical behaviour of EVA|CNT composites studied through in situ NEXAFS spectroscopy**

*Tuesday, August 25, 2015 10:30 AM (20 minutes)***Session Classification:** VI: Material Science

Contribution ID: 93

Type: **not specified**

## **Time-resolved XAFS in kinetic formation and transition mechanism of nanoclusters and nanocrystals**

*Tuesday, August 25, 2015 10:50 AM (20 minutes)***Presenter:** YAO, T.**Session Classification:** VI: Material Science

Contribution ID: 94

Type: **not specified**

**Operando X-ray absorption spectroscopy: A key  
technique to understand the  
structure-function-relationship of noble metal doped  
gas sensing materials**

*Tuesday, August 25, 2015 11:10 AM (20 minutes)*

**Presenter:** DEGLER, D.

**Session Classification:** VI: Material Science

Contribution ID: 95

Type: **not specified**

## **In situ XANES/EXAFS study of the formation of doped and undoped hollow g-Fe<sub>2</sub>O<sub>3</sub> nanoparticles**

*Tuesday, August 25, 2015 11:30 AM (20 minutes)*

**Presenter:** KWON, S.G.

**Session Classification:** VI: Material Science



Contribution ID: 96

Type: **not specified**

## **XFEL-Spectroscopies at XFELs, Short Introduction**

*Tuesday, August 25, 2015 10:30 AM (10 minutes)*

**Presenter:** BRESSLER, C.

**Session Classification:** XEFL

Contribution ID: 97

Type: **not specified**

## **Implications of adding the dimension of time to science with X-rays**

*Tuesday, August 25, 2015 10:40 AM (30 minutes)***Presenter:** FÖHLISCH, A.**Session Classification:** XEFL

Contribution ID: 98

Type: **not specified**

## Orbital-specific mapping of chemical dynamics

*Tuesday, August 25, 2015 11:10 AM (20 minutes)***Presenter:** WERNET, P.**Session Classification:** XEFL

Contribution ID: 99

Type: **not specified**

## Ultrafast generation of magnetic ordering in a first order phase transition in FeRh

*Tuesday, August 25, 2015 11:30 AM (20 minutes)*

**Presenter:** SCHERZ, A.

**Session Classification:** XEFL

Contribution ID: **100**

Type: **not specified**

## **Stimulating soft X-ray emission from condensed matter**

*Tuesday, August 25, 2015 11:50 AM (20 minutes)*

**Presenter:** BEYE, M.

**Session Classification:** XEFL

Contribution ID: **101**Type: **not specified**

## **Homogeneous catalysis and high resolution hard X-ray absorption and emission spectroscopy**

*Tuesday, August 25, 2015 1:30 PM (30 minutes)***Presenter:** BAUER, M.**Session Classification:** III: Advanced Methods

Contribution ID: 102

Type: **not specified**

## **Abrupt vs. gradual spin-crossover in classic Fe(II) and Fe(III) compounds analyzed by high-resolution XAS/XES and DFT**

*Tuesday, August 25, 2015 2:00 PM (20 minutes)***Presenter:** MEBS, S.**Session Classification:** III: Advanced Methods

Contribution ID: **103**Type: **not specified**

## **In situ site-selective K-edge XAS: A powerful probe of the transformation of mixed-valence compounds**

*Tuesday, August 25, 2015 2:20 PM (20 minutes)*

**Presenter:** BORDAGE, A.

**Session Classification:** III: Advanced Methods



Contribution ID: **104**Type: **not specified**

## **Redox sensitivity of cobalt in the CoMoS and CoNiMoS HDS catalyst: a Resonant Inelastic X-ray Scattering study**

*Tuesday, August 25, 2015 2:40 PM (20 minutes)***Presenter:** AL SAMARAI, M.**Session Classification:** III: Advanced Methods

Contribution ID: **105**

Type: **not specified**

## **Looking at one proton with XES**

*Tuesday, August 25, 2015 3:00 PM (20 minutes)*

**Presenter:** MIJOVILOVICH, A.

**Session Classification:** III: Advanced Methods

Contribution ID: **106**Type: **not specified**

## **XAFS in high-energy-density matter: solid iron up to 560GPa**

*Tuesday, August 25, 2015 1:30 PM (30 minutes)***Presenter:** PING, Y.**Session Classification:** V: Radionuclides, actinides, earth and environmental

Contribution ID: 107

Type: **not specified**

## **Structural Properties of Sodium-Rich Carbonate-Silicate Melts: An In-situ High-Pressure EXAFS Study on Y and Sr**

*Tuesday, August 25, 2015 2:00 PM (20 minutes)***Presenter:** POHLENZ, J.**Session Classification:** V: Radionuclides, actinides, earth and environmental

Contribution ID: **108**Type: **not specified**

## **An XAS study of lead speciation in chloride solutions under hydrothermal conditions**

*Tuesday, August 25, 2015 2:20 PM (20 minutes)*

**Presenter:** RAE, N.

**Session Classification:** V: Radionuclides, actinides, earth and environmental

Contribution ID: **109**Type: **not specified**

## **Large area –high spatial resolution iron XANES mapping of impact melt-bearing breccias**

*Tuesday, August 25, 2015 2:40 PM (20 minutes)***Presenter:** WARD, M.J.**Session Classification:** V: Radionuclides, actinides, earth and environmental

Contribution ID: 110

Type: **not specified**

## **Discovering effect of radiation interaction on color of freshwater cultured pearls**

*Tuesday, August 25, 2015 3:00 PM (20 minutes)***Presenter:** PONGKRAPAN, S.**Session Classification:** V: Radionuclides, actinides, earth and environmental

Contribution ID: 111

Type: **not specified**

## **Ex-situ and in-situ investigations of thermal anti-oxidation treatments of Cr-Ni steels by reflection mode EXAFS**

**Presenter:** LÜTZENKIRCHEN-HECHT, D.



Contribution ID: 112

Type: **not specified**

## **Ex-situ and in-situ investigations of thermal anti-oxidation treatments of Cr-Ni steels by reflection mode EXAFS**

*Tuesday, August 25, 2015 1:30 PM (30 minutes)***Presenter:** LÜTZENKIRCHEN-HECHT, D.**Session Classification:** IV: Chemistry, catalysis, operando and time-resolved studies

Contribution ID: 113

Type: **not specified**

**In situ X-ray absorption spectroscopy  
characterization of the incipient growth of ZnO thin  
films by atomic layer deposition**

*Tuesday, August 25, 2015 2:00 PM (20 minutes)*

**Presenter:** CHU, M.-H.

**Session Classification:** IV: Chemistry, catalysis, operando and time-resolved studies

Contribution ID: 114

Type: **not specified**

## **In situ XAFS and XRD observation during a preparation process of an electroluminescent Tb doped alumina film**

*Tuesday, August 25, 2015 2:20 PM (20 minutes)***Presenter:** BANDO, K.K.**Session Classification:** IV: Chemistry, catalysis, operando and time-resolved studies

Contribution ID: 115

Type: **not specified**

## **Atomic structure of PtCu nanoparticles in PtCu/C catalysts prepared by simultaneous and sequential deposition of components on carbon support**

*Tuesday, August 25, 2015 2:40 PM (20 minutes)***Presenter:** BUGAEV, L.A.**Session Classification:** IV: Chemistry, catalysis, operando and time-resolved studies

Contribution ID: 116

Type: **not specified**

## **EXAFS-A Powerful Tool to Determine the Structure of Active Species in Single-atom Catalysts**

*Tuesday, August 25, 2015 3:00 PM (20 minutes)***Presenter:** ZHANG, L.**Session Classification:** IV: Chemistry, catalysis, operando and time-resolved studies

Contribution ID: 117

Type: **not specified**

## **Electrochemical operando soft x-ray emission spectroscopy for Li-ion-battery electrodes**

*Tuesday, August 25, 2015 1:30 PM (20 minutes)***Presenter:** ASAKURA, D.**Session Classification:** VII. Energy-related materials

Contribution ID: **118**Type: **not specified**

## **Operando XAS Characterization of LiS Batteries**

*Tuesday, August 25, 2015 1:50 PM (20 minutes)***Presenter:** GORLIN, Y.**Session Classification:** VII. Energy-related materials

Contribution ID: 119

Type: **not specified**

## **In situ XAS/XRD Study of Li<sub>2</sub>FeSiO<sub>4</sub> as LIB Cathode Material**

*Tuesday, August 25, 2015 2:10 PM (20 minutes)***Presenter:** ARTHUR, Z.**Session Classification:** VII. Energy-related materials



Contribution ID: 120

Type: **not specified**

## **In-situ techniques for soft X-ray spectroscopy on catalytic and electrochemical systems**

*Tuesday, August 25, 2015 2:30 PM (20 minutes)***Presenter:** SCHWANKE, C.**Session Classification:** VII. Energy-related materials

Contribution ID: **121**Type: **not specified**

## Operando XAS study of Li-S batteries

*Tuesday, August 25, 2015 2:50 PM (20 minutes)***Presenter:** AQUILANTI, G.**Session Classification:** VII. Energy-related materials

Contribution ID: 122

Type: **not specified**

## **Probing chemical reaction dynamics with atomic specificity and resolution**

*Tuesday, August 25, 2015 1:30 PM (20 minutes)*

**Presenter:** GAFFNEY, K.

**Session Classification:** XEFL

Contribution ID: 123

Type: **not specified**

## Tracking light-induced ultrafast transformations of transition metal complexes

*Tuesday, August 25, 2015 1:50 PM (20 minutes)***Presenter:** VANKÓ, G.**Session Classification:** XEFL

Contribution ID: 124

Type: **not specified**

## **Developments for time-resolved x-ray spectroscopies using X-ray Free Electron Lasers at SACLA**

*Tuesday, August 25, 2015 2:10 PM (20 minutes)***Presenter:** KATAYAMA, T.**Session Classification:** XEFL

Contribution ID: 125

Type: **not specified**

## **Femto to Picosecond Transient States of a Photoexcited WO<sub>3</sub> Photocatalyst**

*Tuesday, August 25, 2015 2:30 PM (20 minutes)***Presenter:** UEMURA, Y.**Session Classification:** XEFL

Contribution ID: 126

Type: **not specified**

## **Development in Ultrafast X-ray Spectroscopy at the X-ray Pump Probe Instrument of the LCLS**

*Tuesday, August 25, 2015 2:50 PM (20 minutes)***Presenter:** ZHU, D.**Session Classification:** XEFL

Contribution ID: 127

Type: **not specified**

## **Asymmetric pathways in the electrochemical conversion reaction of NiO as battery electrode with high storage capacity**

*Tuesday, August 25, 2015 3:50 PM (20 minutes)***Presenter:** MARCUS, M.**Session Classification:** VII. Energy-related materials



Contribution ID: 128

Type: **not specified**

## **XAS spectroscopic fingerprint of the active site in non-precious metal electrocatalysts for PEM fuel cells**

*Tuesday, August 25, 2015 4:10 PM (20 minutes)***Presenter:** ZITOLO, A.**Session Classification:** VII. Energy-related materials

Contribution ID: 129

Type: **not specified**

## **A XAS study of the local environment and reactivity of Pt-sites in functionalized UiO-67 MOFs**

*Tuesday, August 25, 2015 4:30 PM (20 minutes)*

**Presenter:** BORFECCIA, E.

**Session Classification:** VII. Energy-related materials

Contribution ID: 130

Type: **not specified**

**On the electronic structure and coordination  
geometry of iron based metallo-supramolecular  
coordination polyelectrolytes in working  
electrochromic devices**

*Tuesday, August 25, 2015 4:50 PM (20 minutes)***Presenter:** SZCZERBA, W.**Session Classification:** VII. Energy-related materials

Contribution ID: 131

Type: **not specified**

## **Ground state character in high-resolution x-ray absorption at M, N and O edges of actinides**

*Tuesday, August 25, 2015 3:50 PM (20 minutes)***Presenter:** BUTORIN, S.M.**Session Classification:** V: Radionuclides, actinides, earth and environmental

Contribution ID: 132

Type: **not specified**

## Using X-ray Raman to Study Soil Carbon Biogeochemistry

*Tuesday, August 25, 2015 4:10 PM (20 minutes)***Presenter:** MISHRA, B.**Session Classification:** V: Radionuclides, actinides, earth and environmental

Contribution ID: 133

Type: **not specified**

## **XAFS study of copper(II) diethylenetriamine complexes having different coordination geometries**

*Tuesday, August 25, 2015 4:30 PM (20 minutes)***Presenter:** GAUR, A.**Session Classification:** V: Radionuclides, actinides, earth and environmental

Contribution ID: 134

Type: **not specified**

## **X-Ray Absorption Spectroscopic analyses of stable Fe-phases in aged cements**

*Tuesday, August 25, 2015 4:50 PM (20 minutes)*

**Presenter:** VESPA, M.

**Session Classification:** V: Radionuclides, actinides, earth and environmental

Contribution ID: 135

Type: **not specified**

## **Local structure and bonding of magnetic dopants in Bi<sub>2</sub>Se<sub>3</sub> and Bi<sub>2</sub>Te<sub>3</sub> topological insulator thin films**

*Tuesday, August 25, 2015 3:50 PM (20 minutes)***Presenter:** FIGUEROA, A.**Session Classification:** VI: Material Science



Contribution ID: 136

Type: **not specified**

## **EXAFS study on the structural properties of In and In + C implanted Ge**

*Tuesday, August 25, 2015 4:50 PM (20 minutes)***Presenter:** FENG, R.**Session Classification:** VI: Material Science

Contribution ID: 137

Type: **not specified**

## **Subtle local structural variations in oxygen deficient niobium germanate thin film glasses as revealed by x-ray absorption spectroscopy**

*Tuesday, August 25, 2015 4:10 PM (20 minutes)***Presenter:** SAHINER, M.A.**Session Classification:** VI: Material Science

Contribution ID: 138

Type: **not specified**

## **Soft x-ray absorption spectroscopy on Atomic Layer Deposition grown ZnO films**

*Tuesday, August 25, 2015 4:30 PM (20 minutes)***Presenter:** KOWALIK, I.A.**Session Classification:** VI: Material Science

Contribution ID: 139

Type: **not specified**

## **X-Ray Spectroscopy at XFELs –Present and Future**

*Tuesday, August 25, 2015 3:50 PM (20 minutes)***Session Classification:** XEFL

Contribution ID: 140

Type: **not specified**

## **Revealing charge carrier trapping in ZnO nanoparticles with femtosecond time-resolved X-ray spectroscopy**

*Tuesday, August 25, 2015 4:10 PM (20 minutes)***Presenter:** PENFOLD, T.**Session Classification:** XEFL

Contribution ID: 141

Type: **not specified**

## **RIXS spectroscopy at hard XFELs using non-monochroma-tized SASE pulses**

*Tuesday, August 25, 2015 4:30 PM (20 minutes)*

**Presenter:** KAYSER, Y.

**Session Classification:** XEFL

Contribution ID: 142

Type: **not specified**

## **Matter under extreme conditions probed with ultrafast XANES on FEL facilities**

*Tuesday, August 25, 2015 4:50 PM (20 minutes)***Presenter:** HARMAND, M.**Session Classification:** XEFL

Contribution ID: **143**

Type: **not specified**

## **XFEL-close out**

*Tuesday, August 25, 2015 5:10 PM (10 minutes)*

**Presenter:** BRESSLER, C.

**Session Classification:** XEFL



Contribution ID: 144

Type: **not specified**

## Ultrafast X-ray Spectroscopic Probing of Catalytic Surface Chemical Reactions using LCLS

*Tuesday, August 25, 2015 8:30 AM (20 minutes)*

**Presenter:** NILSSON, Anders

**Session Classification:** II. New sources and new instrumentation

Contribution ID: 145

Type: **not specified**

## **Emerging applications of high-resolution XANES spectroscopy in environmental science**

*Tuesday, August 25, 2015 9:00 AM (40 minutes)***Presenter:** MANCEAU, Alain**Session Classification:** V: Radionuclides, actinides, earth and environmental

Contribution ID: 146

Type: **not specified**

## **XMCD on Fe-based nanoparticles: Two examples of theory and experiment complementing one another**

*Friday, August 28, 2015 10:20 AM (30 minutes)*

**Presenter:** SCHMITZ-ANTONIAK, C.

**Session Classification:** VI: Material Science