

## MONDAY 27

Location: Benedetto XIII

### 8.30 Conference opening

### 9.00/10.30 Plenary session M1

9.00 Sarma D. D.

*EXAFS and NEXAFS studies of strongly correlated electron systems*

9.45 Kotani Akio

*Theoretical and experimental study of high-magnetic-field XMCD spectra at the  $L_{2,3}$  absorption edges of mixed-valence rare-earth compounds*

### 11.00/13.00 Symposium S1

*Electronic correlations, corehole interaction and relaxation effects in x-ray absorption spectra*

11.00 Kruger Peter

*Multiple couplings and band structure in  $L_{2,3}$ -edge absorption through multi-channel multiple scattering theory*

11.25 Taranukhina Anna

*Multichannel Green's function multiple scattering calculations of x-ray absorption*

11.50 Ebert Hubert

*Theoretical description of X-ray absorption in correlated magnetic solids*

12.15 Ikeno Hidekazu

*Ab-initio CI calculations for 3d transition metal  $L_{2,3}$  x-ray absorption spectra*

12.40 Shirley Eric

*Exotic effects in near-edge spectra*

### 11.30/13.30 Poster Session PS1

15.30/17.30 Location: Ducal Palace

#### ■ P1.1 Material Science I Sala La Muta

15.30 Wei Shiqiang

*Experimental and theoretical investigations on ferromagnetic nature of dilute magnetic semiconductors*

15.50 Lawniczak-Jablonska Krystyna

*The influence of high temperature annealing procedures on the location of Mn inside the GaAs matrix*

16.10 Ruffoni Matthew

*Measuring strain at the atomic-scale with Differential X-ray Absorption Spectroscopy*

16.30 Yalovega Galina

*Fluorinated single-walled carbon nanotubes: X-ray absorption and DFT analysis*

16.45 Pedio Maddalena

*Investigation of C K-edge of differently sp-hybridized systems*

17.00 Ouvrard Guy

*In operando characterization of lithium battery materials*

17.15 Arcon Iztok

*In situ XAS studies of new cathode materials for high energy Li-ion batteries*

#### ■ P1.2 Disordered Systems Allara e Grosso

15.30 Ferlat Guillaume

*MD-XAS studies of glasses and liquids: from weakly to highly disordered cases*

15.50 Schnohr Claudia

*Amorphous phase structure and vibrational anisotropy in the III-V semiconductor InP*

16.10 Coppari Federica

*Combined EXAFS and Raman high-pressure studies of amorphous Ge and SiGe alloys*

16.30 Lahiri Debduutta

*Structural understanding of the preferential glass-formation-ability in multi-component bulk metallic glass, using XAFS*

16.45 Kolobov Alex

*EXAFS study of the local structure of liquid*

*Ge<sub>2</sub>Sb<sub>2</sub>Te<sub>5</sub> (GST)*

17.00 Spezia Riccardo

*Molecular dynamics to rationalize EXAFS experiments: a dynamical model explaining hydration behaviour across the lanthanoids(III) series*

17.15 Migliorati Valentina

*Ion hydration in high-density water*

#### ■ P1.3 Instrumentation Aula Aranjo Ruiz

15.30 Frenkel Anatoly

*Combined XAFS/XRD instrument at the X18A beamline at NSLS for in situ, time-resolved catalysis research*

15.50 Fonda Emiliano

*First results at SAMBA the SOLEIL hard x-ray beamline for EXAFS and QEXAFS experiments*

16.10 Kleimenov Evgueni

*HERFD XAS / RIXS spectrometer*

16.30 Rocca Francesco

*Nano-scale X-ray absorption spectroscopy using XEOL-SNOM detection mode*

16.45 Silversmit Geert

*Polycapillary based  $\mu$ -XAS and confocal  $\mu$ -XANES at a bending magnet source of the ESRF*

17.00 Marcelli Augusto

*Time-resolved simultaneous spectroscopies as a probe of physical-chemical processes*

17.15 Zhang Ke

*Very sensitive X-ray fluorescence analyzer detector*

#### ■ P1.4 Theory I Aula Betti

15.30 Fujikawa Takashi

*Relativistic many-body XMCD theory including core degenerate effects*

15.50 Harada Isao

*Theory of XAS and XMCD for field-controlled valence mixed states in RE compounds*

16.10 Hatada Keisuke

*Full potential multiple scattering for core electron spectroscopies*

16.30 Joly Yves

*Self-consistency, Hubbard, spin-orbit and other advances in the FDMNES code to simulate XANES and RXD experiments*

16.50 Sébilleau Didier

*On the convergence of the multiple scattering series*

17.10 Gougoussis Christos

*Parameter free calculations of K-edge XAS in solids: theory and applications*

18.00/20.00 Location: Ducal Palace

#### ■ P2.1 Nano structures I Sala La Muta

18.00 Bianconi Antonio

*Probing fast quantum lattice and charge critical fluctuations by XANES and EXAFS*

18.30 Soo Yun-Liang

*Studies of long-range-order and short-range-order structures in zirconia nanocrystals using TEM, XRD, and EXAFS*

18.45 Carta Daniela

*An X-ray absorption study of the inversion degree in ferrite nanocrystals  $MFe_2O_4$  ( $M = Mn, Co, Ni$ )*

19.00 Dubiel Manfred

*Temperature dependence of EXAFS cumulants of Ag nanoparticles in glasses*

19.15 Requejo Felix

*Structural and electronic characterization of  $Fe_2O_3$  capped Au nanoparticles*

*Charge effects on Au core induced by the Fe-oxide shell.*

19.30 Bitter Harry

*Structure performance relations in nano-sized Ti-doped sodium-alanate for hydrogen storage*

19.45 Maurizio Chiara

*Ag-for-Na ion-exchanged waveguides:*

*correlation between the Ag site and the photoluminescence emission.*

#### ■ P2.2 Extreme conditions Allara e Grosso

18.00 Itié Jean-Paul

*High pressure x-ray absorption spectroscopy: energy dispersive versus classical set-up*

18.20 Baudalet François

*Magnetism and structure under extreme condition*

18.40 Pellicer-Porres Julio

*X-ray absorption study of  $CuGaO_2$  and  $CuAlO_2$  delafossites under high pressure*

19.00 Aquilanti Giuliana

*Melting in the diamond anvil cell using energy dispersive XAS*

19.15 Ramos Aline

*Pressure induced metal-insulator transition in  $LaMnO_3$*

19.30 Pylkkänen Tuomas

*High-pressure ices VI-VIII studied with x-ray Raman scattering*

19.45 Peyrusse Olivier

*K-edge absorption spectra in Warm Dense Matter*

#### ■ P2.3 Chemistry Aula Aranjo Ruiz

18.00 Frank Patrick

*The XAS model of dissolved Cu(II) and its significance to biological electron transfer*

18.30 Giorgetti Marco

*EXAFS and XANES Simulations of Fe/Co hexacyanoferrate spectra by GNXAS and MXAN*

18.45 Tenderholt Adam

*Sulfur K-edge x-ray absorption spectroscopy and density functional theory calculations on molybdenum tris(dithiolene) complexes: XAS as a probe of electronic and geometric structures*

19.00 Provost Karine

*Coupling CP-MD simulations and x-ray absorption spectroscopy: exploring the structure of oxaliplatin in aqueous solution.*

19.15 Jalilehvand Farideh

*Cadmium(II) complex formation with cysteine, penicillamine and glutathione in aqueous solution and solid state*

19.30 Miedema Piter

*2p x-ray absorption of iron and cobalt-phthalocyanines*

19.45 Alonso Mori Roberto

*Electronic structure of sulfur studied by x-ray absorption and emission spectroscopy*

#### ■ P2.4 Theory II Aula Betti

18.00 Bordage Amélie

*$V^{3+}$  incorporation in garnet: experiments and calculations*

18.20 Benfatto Maurizio

*The MXAN analysis of the sulphur K-edge XANES of cysteine*

18.40 Cabaret Delphine

*The use of band structure pseudopotential DFT codes for the calculation of XANES spectra: recent applications in biological materials, minerals and glasses*

19.00 Juhin Amélie

*From local to itinerant model of X-ray Absorption: application to the calculation of X-ray Natural Linear Dichroism*

19.20 Mijovilovich Ana

*Relaxed final state DFT simulations of sulfur K-edge XANES and microXANES for catalysis.*

19.40 Vedrinskii Rostislav

*A new interpretation of  $L_{2,3}$  X-ray absorption in rutile  $TiO_2$ .*