



EUSpec Training School on Multiple Scattering Codes : 27-30 June 2016

- 1st day : theory courses on multiple scattering
(Louis Antoine Hall, Buiding 2)

8h15 - 8h45	Registration + welcome coffee (R. Römling-Engl, E. Robin)
8h45 - 9h00	Welcome of the participants (D. Sébilleau and K. Hatada)
9h00 - 9h45	D. Sébilleau (Rennes) : <i>Introduction to (multiple) scattering theory</i>
9h45 - 10h30	Jan Minár (Munich) : <i>Multiple scattering formalism as a basis for electronic structure calculations</i>
10h30 - 11h00	Coffee break
11h00 - 11h45	K. Hatada (Rennes) : <i>Full potential multiple scattering theory space with space filling cells in real space</i>
11h45 - 12h30	C. R. Natoli (Frascati) : <i>Computing the potential : the phagen_scf code</i>
12h30 - 13h30	Lunch break
13h30 - 14h15	O. Šipr (Prague) : <i>DMFT and multiple scattering theory</i>
14h15 - 15h00	M. Benfatto (Frascati) : <i>MXAN and Molecular Dynamic: a new way to look to the XANES energy region</i>
15h00 - 15h45	A. Di Cicco (Camerino) : <i>X-ray absorption spectroscopy and n-body distribution functions: theoretical background of the GNXAS data-analysis method</i>
15h45 - 16h15	Coffee break + posters installation (posters in rooms 203-204, building 2)
16h15 - 17h00	P. Krüger (Chiba) : <i>Multichannel multiple scattering in R-matrix formalism</i>
17h00 - 17h45	A. Taranukhina (Rostov) : <i>Multiple scattering in Green's function formalism: one channel and multichannel versions</i>

- days 2-4 : training on the computer codes : MXAN (Frascati), GNXAS (Camerino), MsSpec (Rennes), FPMS (Rennes), MCMS (Chiba) : [hands-on in room 250, 2nd floor of building 2, posters in rooms 204-205 and coffee in room 203](#)

	Tuesday the 28th June 2016	Wednesday the 29th June 2016	Thursday the 30th June 2016	
8h30-10h30	Hands-on MXAN -1 : M.Benfatto/E. Pace	Hands-on MsSpec -1 : D. Sébilleau/T. Jaouen	Hands-on MCMS -1 : P. Krüger/A. Koide	WG2-WG5 meeting (organised by B. Brena and M. Pedio) room 207
10h30-11h00	Coffee break/posters	Coffee break/posters	Coffee break/posters	
11h00-12h30	Hands-on MXAN -2 : M.Benfatto/E. Pace	Hands-on MsSpec -2: D. Sébilleau/T. Jaouen	Hands-on MCMS -2: P. Krüger/A. Koide	
12h30-13h30	Lunch break	Lunch break	Lunch break	
13h30-15h30	Hands-on GNXAS -1 : A. Di Cicco/M. Minicucci	Hands-on FPMS -1 : K. Hatada/A. Koide	Hands-on : MXAN, GNXAS, MsSpec, FPMS, MCMS	EUSpec management committee meeting room 207
15h30-16h00	Coffee break/posters	Coffee break/posters	Coffee break/posters	
16h00-17h30	Hands-on GNXAS-2: A. Di Cicco/ M. Minicucci	Hands-on FPMS -2 : K. Hatada/A. Koide	Poster session Best poster prize	
17h30-18h30	Local beers tasting session (Club des Professeurs)	Visit of <i>Parlement de Bretagne</i> at 17h30	Conclusion	
19h00-22h30		Workshop dinner at the <i>Paris-New-York restaurant</i>	Reception at the <i>Town Hall</i> at 18:30	

MSNano conference: 1-2 July 2016

- 1st of July 2016: 4th MSNano workshop : amphitheater M, building 42 (ESIR)

Time	Talk	Chair
8h00 - 8h30	Registration (R. Römling-Engl, E. Robin)	
8h30 - 8h45	Welcome (D. Sébilleau, H. Ebert) Obituaries : W. Temmerman (H. Ebert), Z. Wu (A. Marcelli), W. Kohn (J. J. Rehr)	
8h45 - 9h10	M. Cammarata (Rennes) : <i>Time resolved X-ray absorption Experiments (6 to 18 keV) at Synchrotrons and Free Electron Lasers</i>	K. Hatada
9h10 - 9h35	A. Di Cicco (Camerino) : <i>X-ray absorption with free electron lasers: first results at Fermi@Elettra</i>	K. Hatada
9h35 - 10h00	O. Šipr (Prague) : <i>Full-potential polarized XANES calculation by combining pseudopotential and multiple-scattering methods: A poor-man's solution</i>	A. Gellé
10h00 - 10h25	H. Ebert (Munich) : <i>Inclusion of temperature effects in the calculations of response properties</i>	A. Gellé
10h25 - 10h40	Coffee break	
10h40 - 11h05	C. R. Natoli (Frascati) : <i>Investigation of the ground state of Au-supported FePc Film based on the interpretation of Fe K- and L-edge XMCD</i>	H. Ebert
11h05 - 11h30	P. Krüger (Chiba) : <i>L-edge absorption and dichroism in low symmetry (d0) compounds</i>	H. Ebert
11h30 - 11h55	A. Taranukhina (Rostov on Don) : <i>Multichannel L-absorption calculations by analytic continuation of Green's function onto complex energy plane</i>	H. Ebert
11h55 - 12h50	Lunch break	
12h50 - 13h15	P. Turban (Rennes) : <i>Ballistic Electron Emission Microscopy : hot-electrons for probing interface electronic properties at the nanoscale</i>	T. Fujikawa
13h15 - 13h40	K. Hatada (Rennes) : <i>Multiple scattering theory of BEEM in real space</i>	T. Fujikawa
13h40 - 14h05	C. Godet (Rennes) : <i>Photoelectron energy loss spectroscopy : retrieving the Energy Loss Function from XPS experiments</i>	P. Krüger
14h05 - 14h30	T. Fujikawa (Chiba) : <i>Plasmon losses in core photoemission spectra</i>	P. Krüger
14h30 - 14h55	J. Minár (Munich)/K. Hatada (Rennes)/N. Komiya (Chiba) : <i>The ESL library/ The ES2MS package</i>	P. Krüger
14h55 - 15h10	Coffee break	
15h10 - 15h35	D. Sébilleau (Rennes) : <i>A complete multiple scattering approach to EELS</i>	C. Natoli
15h35 - 16h00	R. Choubisa (Pilani) : <i>Coincidence electron impact ionization processes on atoms and extended targets</i>	C. Natoli
16h00 - 16h25	T. Jaouen (Fribourg) : <i>Layer-resolved Auger electron diffraction study of Mg atom incorporation at MgO/Ag(001) interface</i>	C. Natoli
16h25 - 16h50	W. Chu (Hefei) : <i>Structure-property relationship of nanomaterials for the energy storage and conversion studied by XAS and MS calculations</i>	D. Sébilleau
16h50 - 17h15	C. Zou (Hefei) : <i>The electronic and structural transitions studies of VO₂ epitaxial film by X-ray diffraction and polarized X-ray absorption spectroscopy</i>	D. Sébilleau
17h15 - 17h40	T. Miyanaga (Hirosaki) : <i>XAFS study on luminescent Ag-zeolites</i>	D. Sébilleau
17h40 - 18h40	Round table: <i>How to extend the ideas of the MSNano network and federate multiple scattering at European level?</i> (room 4, building 41)	D. Sébilleau / H. Ebert
18h40 - 19h00	Conclusion (D. Sébilleau, H. Ebert)	

- 2nd of July 2016: **A tribute to Rino Natoli for his 75th birthday**
(amphitheater M, building 42 ---ESIR)

Time	Talk	Chair
8h30 - 9h00	Welcome (D. Sébilleau, A. Di Cicco)	
9h00 - 9h30	F. Palumbo (Frascati) :	C. S. Fadley
9h30 - 9h45	R. Gunnella (Camerino) : <i>Surfaces: structure and soul chez Rino</i>	C. S. Fadley
9h45 - 10h00	K. Hatada (Rennes) : <i>Revolutionary, Innovative, Novel, Outstanding</i>	C. S. Fadley
10h00 - 10h15	S. Di Matteo (Rennes) : <i>Learning from Rino: Sum-Rules, V₂O₃ & Latino</i>	C. S. Fadley
10h15 - 10h30	A. Taranukhina (Rostov on Don) : <i>Multi-aqueduct approach to the interaction with Rino Natoli</i>	C. S. Fadley
10h30 - 10h45	Coffee break	
10h45 - 11h00	P. Krüger (Chiba) : <i>All channels lead to Frascati</i>	J. J. Rehr
11h00 - 11h15	N. Perkins (Minneapolis) : <i>Mott physics with spin-orbit coupling and orbital degeneracy: how the ideas on V₂O₃ lead to the development of a new field in 21st century</i>	J. J. Rehr
11h15 - 11h30	Y. Joly (Grenoble) : <i>Fun with Resonant Diffraction</i>	J. J. Rehr
11h30 - 11h45	K. Palotás (Budapest) : <i>Screened KKR</i>	J. J. Rehr
11h45 - 12h15	C. Brouder (Paris) : <i>Relativistic effects and gauge invariance in x-ray spectroscopy and scattering</i>	J. J. Rehr
12h15 - 13h30	Lunch break	
13h30 - 14h00	C. S. Fadley (Berkeley) : <i>Some new developments in the study of bulk materials and buried interfaces with photoemission, and some challenges for theory</i>	N. Perkins
14h00 - 14h30	J. J. Rehr (Seattle) : <i>Theory of inelastic losses and satellites in x-ray spectra</i>	N. Perkins
14h30 - 15h00	M. A. Van Hove (Hong-Kong) : <i>Large molecules on metal surfaces: from C₆₀ to molecular motors</i>	N. Perkins
15h00 - 15h30	H. Daimon (Nara) : <i>3D atomic structure analysis around local active atoms by two-dimensional photoelectron diffraction and holography</i>	N. Perkins
15h30 - 15h45	Coffee break	
15h45 - 16h00	H. Ebert (Munich) : <i>Relativistic multiple scattering calculations in the full-potential mode</i>	M. A. Van Hove
16h00 - 16h15	R. Zeller (Jülich) : <i>Precise large-scale density-functional calculations</i>	M. A. Van Hove
16h15 - 16h30	P. Sainctavit (Paris): <i>Quantum tunnelling of magnetization and Single Molecule Magnets</i>	M. A. Van Hove
16h30 - 16h45	A. Marcelli (Frascati) : <i>From the MS ideas to the experimental determination of a three-body correlation function using XAS</i>	M. A. Van Hove
16h45 - 17h00	G. Stefani (Rome) : <i>Do pairs of electrons diffract as a whole</i>	M. A. Van Hove
17h00 - 17h15	O. Šipr (Prague) : <i>Influence of spin-orbit coupling on the magnetic dipole term Tz</i>	H. Daimon
17h15 - 17h30	J. García (Zaragoza) : <i>Local Geometry by XAS and RXS</i>	H. Daimon
17h30 - 17h45	T. Fujikawa (Chiba) : <i>Theory of pump-probe ultrafast XPS</i>	H. Daimon
17h45 - 18h00	M. Pedio (Trieste) : <i>Full Multiple Scattering applied to XAS of molecular solids</i>	H. Daimon
18h00 - 18h15	J. Minár (Munich/Plzeň) : <i>Multiple scattering meets correlations</i>	H. Daimon
18h15 - 18h30	Conclusion : C. R. Natoli	

19h30 - 23h30	Conference dinner : garden party in Montrou	
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