

Workshop and hands-on school on the FP-LMTO method and DMFT

June 4-8, 2018 – Santo Stefano di Sessanio (AQ), Italy

Scientific Program

	Monday	Tuesday	Wednesday	Thursday	Friday
09:00		Johan Schött	Samara Keshavarz	Patrik Thunström	Weiwei Sun
09:45		Jindrich Kolorenc	Lars Nordström	Michael Sekania	D. Wang / H. Ullah
10:30	Introduction	Coffee Break	Coffee Break	Coffee Break	Coffee Break
11:00	John Wills	Akihiro Koide	Gianni Profeta	Arya Subramonian	Developers
11:45	Ann Mattson	Mebarek Alouani	Lars Eriksson	Saleem Ayaz Khan	Final remarks
12:30	Lunch	Lunch	Lunch	Lunch	Lunch
14:00	Barbara Brena	Jan Minar	Excursion	Silvia Picozzi	Tutorial only
14:45	Diana Iușan	Iulia Brumboiu	Excursion	Biplab Sanyal	Tutorial only
15:30	Coffee Break	Coffee Break	Excursion	Coffee Break	Coffee Break
16:00	Leonid Pourovskii	Heike Herper	Excursion	Developers	Tutorial only
16:45	Anna Delin	Olga Vekilova	Excursion	Developers	Tutorial only

Topics: Spectroscopy Magnetism FP-LMTO Materials Low dimensions Strong correlations

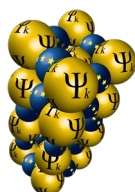
Tutorials

The RSPt tutorials will be held in a dedicated room from Monday to Friday, 14:00-17:30, in parallel with the afternoon scientific sessions. Afternoon coffee breaks will be shared by all attendants. Tutorials attendants should bring their own laptop and make sure to have appropriate software for remote connections. The tutorials from Monday to Thursday will cover basic and advanced usage of RSPt. The Friday session, instead, will be dedicated to problems brought by attendants, i.e. examples of calculations which they intend to make with RSPt. Support will also be offered for compiling RSPt on external supercomputers.

Further information

On Thursday and Friday there will be 2 sessions explicitly dedicated to RSPt developments, in order to discuss various technical issues, such as new input, new features, et cetera. All participants are warmly invited to join the Wednesday excursion, which will be followed by a social dinner.

Acknowledgments



Monday

John Wills	An introduction to FP-LMTO and RSPT
Ann Mattsson	A density based Electron Localization Function
Barbara Brena	Single molecule magnets: spin manipulation, intermolecular interactions and electronic structure. An overview by ab-initio calculations and beyond
Diana Iuşan	Spin-lattice dynamics from first-principles
Leonid Pourovskii	Localized systems within DFT+Hubbard-I approach: multiplets, crystal-field effects and inter-site exchange interactions
Anna Delin	High throughput calculations applied to double perovskites

Tuesday

Johan Schött	XAS for strongly correlated systems
Jindrich Koleček	Theory of resonant x-ray emission spectra at the L and M edges in compounds with localized f electrons
Akihiro Koide	Spin-orbit interaction in light element K-edge XMCD
Mebarek Alouani	From an LMTO to a PAW basis set: a GW implementation
Jan Minar	Understanding of dynamics of excited states by means of static one-step model of ARPES
Iulia Brumboiu	Valence photoionization beyond the electric dipole approximation: the case of $[\text{Ni}(\text{H}_2\text{O})_6]^{2+}$
Heike Herper	Itinerant or localized? – How we can predict the nature of 4f states in Ce-compounds
Olga Vekilova	Magnetic anisotropy of Fe ₃ Sn-based magnets: a first-principles RSPT study

Wednesday

Samara Keshavarz	Electronic structure, magnetism, and exchange integrals in transition-metal oxides: Role of the spin polarization of the functional in DFT+U calculations
Lars Nordström	Currents and spin-currents in non-collinear magnets
Gianni Profeta	Chiral Spin Texture in the Charge-Density-Wave Phase of the Correlated Metallic Pb/Si (111) Monolayer
Lars Eriksson	Enhancing low quality crystal structures and predicting new crystal structures with solid state calculations

Thursday

Patrik Thunström	Probing the topological nature of SmB ₆ using DFT+DMFT in RSPT
Michael Sekania	Scaling behavior of the Compton profile of elemental metals
Arya Subramonian	Two-particle self-consistent method (TPSC) for the Hubbard model on the honeycomb lattice
Saleem Ayaz Khan	Magnetocrystalline anisotropy of FePt: LDA+DMFT study
Silvia Picozzi	Electrical control of spin-texture in non-magnetic ferroelectrics
Biplab Sanyal	Complexities at oxide interfaces

Friday

Weiwei Sun	The theoretical path of uncovering new stackings in 2D-Mo ₂ C and their electronic and vibrational properties
Duo Wang	Spin-spiral dispersion and magnon-phonon interactions in gamma-Fe
Hamid Ullah	Monolayer platinum dichalcogenides with promising applications in solar cell