# 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 Iuşan | 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

RSPt
Gran Sasso Monti della Laga Parco Nazionale
VERITAS NATURAE

## 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

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| Johan Schött | XAS for strongly correlated systems |
| Jindrich Kolorenc | 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 [Ni(H2O)6]2+ |
| Heike Herper | Itinerant or localized? – How we can predict the nature of 4f states in Ce-compounds |
| Olga Vekilova | Magnetic anisotropy of Fe3Sn-based magnets: a first-principles RSPT study |

## Wednesday

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| 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

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| Patrik Thunström | Probing the topological nature of SmB6 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

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| Weiwei Sun | The theoretical path of uncovering new stackings in 2D-Mo2C 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 |