

PROGRAM

9:30 *Welcome Coffee*

10:00 Opening

Pierangelo Gröning (Empa)

10:15 *Realistic Material Design & Simple Computational modeling closed-loop in an industrial environment*

Patrice Bujard (BASF)

Presentation of ongoing projects from the first call

10:45 *Functional Oxides: Growth, characterisation and reactivity*

Claudia Cancellieri (Empa)

11:00 *RNiO₃ perovskites: exploring the boundary between localized and itinerant behaviour*

Marisa Medarde (PSI)

11:15 *Time-resolved XAS to verify mechanisms of photocatalytic reactions*

Grigory Smolentsev (PSI)

11:30 *Novel oxynitrides for visible-light-driven photoelectrochemical water splitting*

Si Wenping (PSI)

12:00 Lunch Break

13:30 *Computational Design of Novel Materials for Energy Storage Applications"*

Teodoro Laino (IBM)

Short Talks presenting project ideas

14:00 *Theoretical study of photocatalysis on perovskite oxynitrides*

Ulrich Aschauer (ETHZ/Uni BE)

14:10 *Realisation of the Kitaev model in strongly spin orbital coupled systems with three-fold connectivity*

Alun Biffin (PSI)

14:20 *Two-dimensional boron structures*

Stefan Goedecker (Uni BS)

14:30 *Probing weak interactions in low dimensional materials*

Oliver Gröning (Empa)

14:40 *Materials Design at the Nanoscale using Combinatorial Deposition Techniques*

Johann Michler (Empa)

14:50 *Electronic structure of TMO interfaces by soft-X-ray ARPES*

Vladimir Strocov (PSI)

15:00 *Experimental test of a recent model for superconductivity in doped SrTiO₃*

Dirk Van der Marel (Uni GE)

15:10 Coffee Break

15:45 *Transmission electron microscopy of complex oxides for energy applications*

Rolf Erni (Empa)

Short Talks presenting project ideas

16:15 *Atomic scale characterisation of material interfaces using transmission electron microscopy*

Yucheng Zhang (Empa)

16:20 *Chiral separation and chiral sensitive synthesis at architected surfaces*

Thomas Jung (PSI)

16:30 *Na-ion batteries: new challenges*

Claire Villevieille (PSI)

16:40 *Angle-resolved Photoemission spectroscopy (ARPES) on topological semimetals*

Ming Shi (PSI)

16:50 Closing Remarks and End of the Workshop

PARTICIPANTS

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