

Program NCCR MARVEL – Second Experimental verification workshop

23 October 2015, 10:00 – 17:00

Place: Empa Dübendorf,

Room: Theodor Erismann Auditorium (VE102, Verwaltungsgebäude)

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| 10:00 | <i>Welcome / Short Introduction</i> | Pierangelo Gröning (Empa) |
| 10:15 | <i>Realistic Material Design & Simple Computational modeling closed-loop in an industrial environment</i> | Patrice Bujard (BASF) |

Presentation of ongoing projects from the first call

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| 10:45 | <i>Functional Oxides: Growth, characterisation and reactivity</i> | Claudia Cancellieri (Empa) |
| 11:00 | <i>RNiO₃ perovskites: exploring the boundary between localized and itinerant behaviour</i> | Marisa Medarde (PSI) |
| 11:15 | <i>Time-resolved XAS to verify mechanisms of photocatalytic reactions</i> | Grigory Smolentsev (PSI) |
| 11:30 | <i>Novel oxynitrides for visible-light-driven photoelectrochemical water splitting</i> | Si Wenping (PSI) |

12:00 Lunch Break

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| 13:30 | <i>Computational Design of Novel Materials for Energy Storage Applications"</i> | Teodoro Laino (IBM) |
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Short Talks presenting project ideas

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| 14:00 | <i>Theoretical study of photocatalysis on perovskite oxynitrides</i> | Ulrich Aschauer (ETHZ/Uni BE) |
| 14:10 | <i>Realisation of the Kitaev model in strongly spin orbital coupled systems with three-fold connectivity</i> | Alun Baffin (PSI) |
| 14:20 | <i>Two-dimensional boron structures</i> | Stefan Goedecker (Uni BS) |
| 14:30 | <i>Probing weak interactions in low dimensional materials</i> | Oliver Gröning (Empa) |
| 14:40 | <i>Materials Design at the Nanoscale using Combinatorial Deposition Techniques</i> | Johann Michler (Empa) |
| 14:50 | <i>Electronic structure of TMO interfaces by soft-X-ray ARPES</i> | Vladimir Strocov (PSI) |
| 15:00 | <i>Experimental test of a recent model for superconductivity in doped SrTiO₃</i> | Dirk Van der Marel (Uni GE) |

15:10 Coffee Break

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| 15:45 | <i>Transmission electron microscopy of complex oxides for energy applications</i> | Rolf Erni (Empa) |
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Short Talks presenting project ideas

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| 16:15 | xxx | Thomas Jung (PSI) |
| 16:25 | <i>Na-ion batteries: new challenges</i> | Claire Villevieille (PSI) |
| 16:35 | <i>Angle-resolved Photoemission spectroscopy (ARPES) on topological semimetals</i> | Ming Shi |
| 16:45 | Closing Remarks and End of the Workshop | |