

MARVEL PP7 Day Thursday, 3. March 2016 at PSI

Participants: PIs, Postdocs and PhDs of the PP7 projects (Experiment and theory partners). PIs of other Marvel projects (VP1, VP2, HP3, HP4, HP5, and PP6).

Presentations: Each project should present status, results and future plans. I suggest using the outline of the yearly report (see below) as an orientation for the content, try to define an objective for the next year (one for the theory part, one for the experiment part). Projects which have not yet started should present the idea and future plans. An important point is that we show the synergies and feedback loops between theory and experiment. Therefore it is expected that the contributions of the theory part and of the experiment are clearly presented.

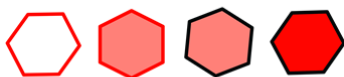
There should be one presentation (or poster) for the experimental part and one for the theory part. Please coordinate yourself between the theory and the experimental partner for each subproject whether you prefer a poster or an oral presentation. For the presentation I suggest that there are two talks for the project, e.g. one 15 min Experiment and one 15 min Theory (plus 10 min discussion), but it is up to the projects to decide how to present in a best way the project and the feedback loop.

Please register via this webpage http://indico.psi.ch/event/MARVEL_PP7day_2016

Deadline for registration: 18.02. 2016, Contact: frithjof.nolting@psi.ch

Agenda, v 2.3.2016

9:30-10:00	Welcome Coffee		WHGA/001
10:00 – 10:10	Short introduction	Frithjof Nolting/Michel Kenzelmann	WHGA/001
10:10-10:50	Theory and Experiment Synergy for Artificial Photosynthesis	Joint presentation: Wenping Si (Exp, PSI) Ivano Castelli (Theory, EPFL)	WHGA/001
10:50-11:30	Development of advanced electrocatalysts for water splitting: Correlation between electronic structure, surface properties and electrochemical activity	Thomas Schmidt (Exp, PSI) Ivano Castelli (Theory, EPFL)	WHGA/001
11:30-12:10	Testing ultrafast processes in condensed matter	Michael Porer (Exp, PSI) Philipp Werner (Theory, UFribourg)	WHGA/001
12:10-13:00	Lunch		WHGA/001
13:00-13:40	RNiO ₃ perovskites: exploring the boundary between localized and itinerant behavior	Dariusz Gawryluk (Exp, PSI) Alexander Hampel (Theory, ETHZ) Oleg Peil (Theory, UGeneva)	WHGA/001
13:40-14:20	Experimental Realization of Novel Topological Semi-metals	Nan Xu (Exp, PSI) Gabriel Autes (Theory, EPFL)	WHGA/001
14:20-14:45	Reserve for discussions		WHGA/001
14:45-16:15	Poster session with Coffee	All other projects, each experiment and theory, additional posters are welcome	SLS entrance hall
16:15-17:00	Closing session of PIs		WSLA/008 (SLS)



	(wrap up and open questions)		
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Outline scientific report

1.1 Scientific goals; Brief description of the short- and long-term research goals.

1.2 Results obtained since the last report

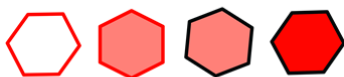
1.3 Planned research for next year

Poster presentations related to one of the running PP7 projects:

	Experiment PI	Experimental poster	Theory poster
Time-resolved X-ray absorption spectroscopy to investigate mechanisms of photochemical water splitting reactions with molecular catalysts	Grigory Smolentsev	Grigory Smolentsev (PSI)	Florian Hodel (Uni ZH)
Microscopic Origin of the Magnetoelectric Properties in Strained and Doped Aurivillius Phases Predicted by DFT	Marta D. Rossell	Marta D. Rossell (EMPA), Claude Ederer (ETHZ)	
The search for new proton conductors: High-throughput screening and experimental synthesis and characterization	Daniele Pergolesi	Daniele Pergolesi (PSI)	Aris Marcolongo (EPFL)
Structural and in-situ electrochemical characterization of oxide phase transformation at oxide-liquid interface	Claudia Cancellieri (EMPA)	Fabio Evangelisti (EMPA)	???
Higgs and Goldstone modes in hexagonal manganites	Dirk van der Marel (U Geneva)	Adrien Stucky (UGeneva)	Quintin Meier (ETHZ)
Resonant Inelastic X-Ray Scattering on thin films and oxide heterostructures for future Mottronics and Orbitronics	Thorsten Schmitt (PSI)	Daniel McNally (PSI)	???

Poster presentations not directly related to one of the running PP7 project

		Experimental poster	Theory poster
Group of Oleg Yazyev			Vamshi Katukuri (EPFL)
Group of Oleg Yazyev			Daniel Gosalbez Martinez (EPFL)



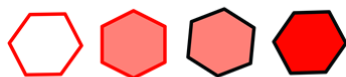
PP7 project which are not yet presented

	Experiment PI	Experimental poster	Theory poster
Using computational chemistry to predict the performance of metal-organic frameworks catalysis in the hydroformylation of olefins	Marco Ranocchiari (PSI)		
Single-band Hubbard Model in New Fluorides	Christian Rüegg (PSI/Uni Geneva)		
Colloidal Nanocrystals as Model Systems to Uncover Structure/Properties Relations in CO ₂ electroreduction	Raffaella Buonsanti (EPFL)	Cannot come	

So far registered:

Autes	Gabriel
Balatsky	Alexander
Cancellieri	Claudia
Castelli	Ivano Eligio
Ederer	Claude
Evangelisti	Fabio
Favre-	
Quattropani	Lidia
Gawryluk	Dariusz Jakub
Gosabez	
Martinez	Daniel
Hampel	Alexander
Hodel	Florian
Hoermann	Nicolas
	Vamshi
Katukuri	Mohan
Kenzelmann	Michel
Lee	Hyungjun
Lippert	Thomas
Luber	Sandra
Marcolongo	Aris
Marzari	Nicola
McNally	Daniel
Medarde	Marisa
Meier	Quintin
Nolting	Frithjof
Peil	Oleg
Pergolesi	Daniele
Porer	Michael

MARVEL



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Rossell	Marta D.
Rüegg	Christian
Schmitt	Thorsten
Shi	Ming
Si	Wenping
Smolentsev	Grigory
Spaldin	Nicola
Staub	Urs
Stucky	Adrien
van der Marel	Dirk
Van Landuyt	Pascale
Werner	Philipp
Xu	Nan