

REPORT ON WORKSHOP:

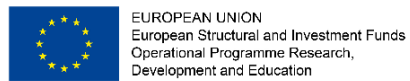
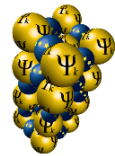
Theory Meets Experiment in Low-Dimensional Structures with Correlated Electrons

Villa Lanna, Prague, Czech Republic, July 1-4, 2019

Organizers: Jan Minar, Jindrich Kolarenc, Pavel Jelinek

Webpage: <https://nano-prg2019.fzu.cz>

Support and funding:



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Introduction

This four-day workshop brought together theorists and experimenters who work on strongly correlated nanosystems adsorbed on surfaces, or on strongly correlated electrons in general. The aim of the event was to exchange ideas and discuss perspectives and future directions of characterization and description of strongly correlated nanosystems. The topics of this workshop included:

- single-atom and single-molecule magnets, magnetic anisotropy
- transport through nanostructures in and out of the linear-response regime
- tuning the electronic properties via interaction with external stimuli or with a substrate
- scanning-probe methods
- electronic structure theory
- advanced valence-band and core-level spectroscopies and their interpretation



Scientific program

The whole Monday 1st of July, was devoted to the experimental techniques used to study nanosystems adsorbed on the surface. Workshop started by introductory talk of H. Brune about the zero dimensional magnetic structures with correlated electrons. In particular the important trend in the experimental community towards correlated f-electron atoms and clusters deposited on the surfaces was shown. These systems shows unique intra-atomic spin-excitations and has been studied by XMCD. Alexander Ako Khajetoorians continued this topic finding the glassy nature of the magnetic state of Nd, where by using spin-polarized scanning tunneling microscopy down to mK temperature, he visualized the competing local non-collinear order at the atomic-scale and probed the subsequent aging phenomena in response to variable magnetic field and temperature. Sander Otte showed the ability to build structures atom-by-atom by means of STM in order to tune the anisotropy and coupling of magnetic atoms on a thin insulators.

Alternative way to the density functional theory which is often used to describe molecular systems has been presented by Ondřej Maršálek. The methodology based on the path integral formulation of quantum mechanics was used to molecular dynamics simulations of aqueous solutions and small molecular clusters at both ambient and low temperatures. Nacho Pascual discussed creation of bound states inside the superconducting gap, named Yu-Shiba-Rusinov states caused by several atomic and molecular impurities.

All invited experimental talks has been supplemented by corresponding theoretical investigations as presented in numerous contributed talks of young early stage researchers.

Every talk was followed by very lively discussion which was not so obvious due to the extraordinary hot day in Prague. This discussion then continued during a welcome reception in Villa Lanna after the last Monday session.

The morning session of Tuesday 2nd was dedicated the teoretical description of single molecule transport. Ferdinand Evers discussed quantum interference and topology in conjugate organic molecules. Inelastic effect in the differential conductance due to the braking of the degeneracy in correlated two-level system was presented by Nicolas Lorente. This effect can be observed by so called isospin-flip spectroscopy. The afternoon session was devoted to the non-trivial spin correlation in 2D graphene based nanostructures (J. Fernández-Rossier) and superlattice TMDCs materials (T. Wehling).

On Wednesday morning, the need of new ab-initio theoretical methods which can describe correlated organometallic ferromagnets and XMCD was formulated by H. Wende. Certainly, one route how finally solve this problem the combination of local density approximation (LDA) and dynamical mean-field theory (DMFT) as presented by Atsushi Hariki. Matthieu Verstraete discussed consequences of thermal vibrations on the electronic and magnetic properties of bulk and nanostructured materials by means of density perturbation theory and alloy analogy CPA model. Exciting new experimental technique to direct image orbitals in correlated oxides has been presented by Hao Tjeng. This application of inelastic X-Ray scattering can certainly help to answer the question of best local orbital in the DMFT and LDA+U.

Scientific discussions obviously continued until and during the social dinner.

The last day of the workshop was devoted to the ultra-fast non-equilibrium phenomena. Jascha Repp presented new developments in the Thz-STM which enable the combination of femtosecond and sub-angstrom resolution in observing reactions of individual molecules directly. With this topic are closely connected two particle excitations. Jan Kunes intorduced dynamical mean-field calculations of collective modes in excitonic magnets. Finally, in the last invited talk of the workshop Sasha Shick reported on more surprises in f-electron systems by means of DFT+U+ED method. With this talk he showed several possible ways how to treat f-electron nanosystems, topic with which the whole workshop started.

We had an balanced ratio of excellent speakers on the side of theory and of experiment. It was clear from the discussions after talks and at the coffee breaks and lunches that the combination of theory and experiment leads to very interesting new ideas.

List of Participants



In
total
the

workshop had 54 participants with 17 invited speakers.

Invited contributions

- Harald Brune (EPF Lausanne, Switzerland)
Zero-Dimensional Magnetic Structures with Correlated Electrons
- Igor Di Marco (APCTP, South Korea)
Ab-initio treatment of the Lanthanides: from solids to clusters and atoms
- Ferdinand Evers (U Regensburg, Germany)
Aspects of Topology and Quantum Interference in Single Molecule Transport
- Joaquín Fernández-Rossier (INL Braga, Portugal)
Spin correlations in graphene nanostructures probed with STM
- Atsushi Hariki (TU Wien, Austria)
LDA+DMFT approach to resonant inelastic x-ray scattering in correlated materials
- Alexander Ako Khajetoorians (Radboud University, Nijmegen, Netherlands)
Unraveling the glassy nature of the magnetic state of Nd
- Jan Kuneš (TU Wien, Austria)
Towards predictive theory of two-particle spectroscopies in strongly correlated materials
- Nicolas Lorente (CSIC-EHU, San Sebastian, Spain)
Isospin-flip spectroscopy
- Ondrej Maršálek (Charles University, Czech Republic)
Nuclear quantum effects in molecular systems through path integrals
- Sander Otte (Delft, Netherlands)
Quantum simulation through atomic assembly
- J. I. Pascual (nanoGUNE, San Sebastian, Spain)
Mapping Yu-Shiba-Rusinov states in atomic and molecular impurities

- Jascha Repp (U Regensburg, Germany)
Actuating and probing a single-molecule switch at femtosecond timescales
- Alexander Shick (Czech Academy of Sciences, Prague, Czech Republic)
More surprises in f-electron magnetism
- Liu Hao Tjeng (Max Planck - CPfS, Dresden, Germany)
Direct Imaging of Orbitals using Inelastic X-Ray Scattering
- Matthieu Verstraete (U Liège, Belgium)
Thermal displacements in microscopies and spectroscopies
- Tim O. Wehling (U Bremen, Germany)
Interactions in superlattice quantum materials
- Heiko Wende (U Duisburg-Essen, Germany)
Europium cyclooctatetraene nanowire carpets: a low-dimensional, organometallic ferromagnet

name	affiliation
Simona Achilli	Catalan Institute of Nanoscience and Nanotechnology, Barcelona, Spain
Fatima Alarab	University of West Bohemia, Czech Republic
Valerio Bellini	CNR - Istituto Nanoscienze, Modena, Italy
Claudio Bonizzoni	Università di Modena e Reggio Emilia, Modena, Italy
Harald Brune	EPFL, Lausanne, Switzerland
Luiza Buimaga-Iarinca	INCDTIM, Cluj-Napoca, Romania
Aleš Cahlík	Institute of Physics, Czech Academy of Sciences, Czech Republic
Gonçalo Catarina	International Iberian Nanotechnology Laboratory, Portugal
Ricardo Ortiz Cano	University of Alicante, Spain
Banhi Chatterjee	Institute of Physics, Czech Academy of Sciences, Czech Republic
Jayita Chakraborty	IISER Bhopal, India
Igor Di Marco	APCTP, Pohang, South Korea
S. W. Dsouza	University of West Bohemia, Czech Republic
Ferdinand Evers	University of Regensburg, Germany
Joaquín Fernández Rossier	INL, Braga, Portugal
Guido Fratesi	University of Milano, Italy
Atsushi Hariki	TU Wien, Austria
Alexander Herman	Universität Duisburg-Essen, Germany
Henning Janßen	IAS-1 FZ Jülich, Germany
Pavel Jelínek	Institute of Physics, Czech Academy of Sciences, Czech Republic
Alžběta Kadlecová	Univerzita Karlova, Czech Republic

Alexander Ako Khajetoorians	Radboud University, Netherlands
Jindřich Kolorenč	Institute of Physics, Czech Academy of Sciences, Czech Republic
Richard Korytár	Charles University, Czech Republic
Peter Kratzer	University Duisburg-Essen, Germany
Juraj Krempasky	Paul Scherrer Institut, Villigen, Switzerland
Vipin Kumar	University of Ulsan, Ulsan, Republic of Korea
Jan Kuneš	TU Wien, Austria
Nicolas Lorente	CSIC, San Sebastian, Spain
Ondřej Maršálek	Charles University, Czech Republic
Jan Minár	University of West Bohemia, Czech Republic
Pingo Mutombo	Institute of Physics, Czech Academy of Sciences, Czech Republic
Tomáš Novotný	Charles University, Czech Republic
Sander Otte	Delft University of Technology, Netherlands
Nacho Pascual	nanoGUNE, San Sebastian, Spain
Michele Pizzochero	EPFL, Lausanne, Switzerland
Vladislav Pokorný	Charles University, Czech Republic
Stéphane Pons	ESPCI Paris - CNRS, France
Indukuru Ramesh Reddy	National Institute of Technology Karnataka, India
Jascha Repp	University of Regensburg, Germany
Ali Sadeghi	Shahid Beheshti University, Iran
Jakub Schusser	University of West Bohemia, Czech Republic
Alexander Shick	Institute of Physics, Czech Academy of Sciences, Czech Republic
Ondřej Šipr	Institute of Physics, Czech Academy of Sciences, Czech Republic
Martin Švec	Institute of Physics, Czech Academy of Sciences, Czech Republic
Evgenia Tereshina-Chitrova	Institute of Physics, Czech Academy of Sciences, Czech Republic
Liu Hao Tjeng	Max Planck – CPfS, Dresden, Germany
Haleem Ud Din	Humboldt University, Berlin, Germany
Hamid Ullah	University of Ulsan, South Korea
Matthieu Verstraete	University of Liege, Belgium
Christian Wäckerlin	Institute of Physics, Czech Academy of Sciences, Czech Republic

Mathias Winder	TU Wien, Austria
Tim Wehling	University of Bremen, Germany
Heiko Wende	University of Duisburg-Essen, Germany

4 Workshop Program

The program featured invited talks from established leaders in the field and from emerging early career researchers in the area. We scheduled 5-10 minutes for questions after every presentation, and this prompted lively discussion and debate.

Monday, July 1			Tuesday, July 2			Wednesday, July 3			Thursday, July 4		
start	length	activity	start	length	activity	start	length	activity	start	length	activity
09:00	00:10	workshop opening	<i>chairman: P. Kratzer</i>			<i>chairman: J. I. Pascual</i>			<i>chairman: M. Švec</i>		
<i>chairman: J. Kuneš</i>			09:00	00:35	F. Evers	09:00	00:35	H. Wende	09:00	00:35	J. Repp
09:10	00:35	H. Brune	09:35	00:20	V. Pokorný	09:35	00:20	Ch. Wackerlin	09:35	00:20	C. Bonizzoni
09:45	00:20	V. Bellini	09:55	00:20	A. Cahlik	09:55	00:20	A. Herman	09:55	00:20	J. Schusser
10:05	00:20	I. R. Reddy	10:15	00:30	coffee break	10:15	00:30	coffee break	10:15	00:30	coffee break
10:25	00:30	coffee break	<i>chairman: H. Brune</i>			<i>chairman: M. Verstraete</i>			<i>chairman: A. Shick</i>		
<i>chairman: T. Novotný</i>			10:45	00:35	N. Lorente	10:45	00:35	M. Verstraete	10:45	00:35	J. Kuneš
10:55	00:35	A. Khajetoorians	11:20	00:20	R. Ortiz	11:20	00:20	H. Ullah	11:20	00:20	G. Fratesi
11:30	00:20	S. W. DSouza	11:40	00:20	T. Novotný	11:40	00:20	S. Achilli	11:40	00:20	E. Tereshina-Chitrova
11:50	00:20	J. Chakraborty	12:00	02:00	lunch	12:00	02:00	lunch	12:00	02:00	lunch
12:10	02:00	lunch	<i>chairman: F. Evers</i>			<i>chairman: J. Kolorenc</i>			<i>chairman: J. Repp</i>		
<i>chairman: H. Wende</i>			14:00	00:35	J. Fernández-Rossier	14:00	00:35	L. H. Tjeng	14:00	00:35	A. Shick
14:10	00:35	A. F. Otte	14:35	00:20	M. Švec	14:35	00:20	O. Šjpr	14:35	00:20	P. Kratzer
14:45	00:20	R. Korytár	14:55	00:20	L. Buimaga-Iarinca	14:55	00:20	A. Sadeghi	14:55	00:20	V. Kumar
15:05	00:35	O. Maršálek	15:15	00:30	coffee break	15:15	00:30	coffee break	15:15	00:30	coffee break
15:40	00:30	coffee break	<i>chairman: R. Korytár</i>			<i>chairman: L. H. Tjeng</i>			<i>chairman: I. Di Marco</i>		
<i>chairman: J. Fernández-Rossier</i>			15:45	00:35	T. Wehling	15:45	00:35	A. Hariki	15:45	00:20	H. Janssen
16:10	00:35	J. I. Pascual	16:20	00:20	M. Pizzochero	16:20	00:20	M. Winder	16:05	00:20	F. Alarab
16:45	00:20	S. Pons	16:40	00:20	H. Ud Din	16:40	00:20	B. Chatterjee	16:25		workshop closing
17:05	00:20	A. Kadlecová	17:00	00:20	J. Krempaský						

5 Abstracts

The workshop received a very positive feedback from invited lecturers and attendees. The book of abstracts can be find under following link:

<https://nano-prg2019.fzu.cz/abook.pdf>