

Report on the Psi-k/CECAM Research Conference “Ab initio Spin-Orbitronics”

September 25, 2017 - September 29, 2017
Hotel Promenade, Montesilvano, Pescara (Italy)

Organizers:

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Introduction

The main purpose of this Psi-k/CECAM research conference (with about 110 participants) has been to highlight the very recent theoretical and computational developments related to the interplay of spin-orbit interaction with electronic structure, magnetism, transport as well as its link to strongly correlated materials and ultrafast currents in diverse materials. We have focused on discussing spin-orbit coupling (SOC) as a means of engendering fundamentally novel physical phenomena in exotic systems. The Conference therefore spanned several research dimensions, ranging from Materials (in the form of bulk compounds, surfaces and interfaces, thin films and heterostructures) to Functionalities (associated with topology, spin-momentum locking, valley degrees of freedom, skyrmions, coupling to electric currents by Berry phases, etc.) to method developments (in terms of dynamical processes in out-of-equilibrium quantum matter, Berry phase physics, etc). A brainstorm about concepts and ideas in a little understood phenomenon, such as orbital magnetization, was carried out under the guidance of Prof. Ivo Souza. While the main focus was on *ab initio* simulations, a few leading scientists in experiments were invited (Prof. Stuart Parkin, Prof. Claudia Felser, etc) and a strong interface to many-body physics treated on the basis of realistic model Hamiltonians was included.

Major outcomes

The 10 major scientific points discussed at the meeting were addressed in the corresponding sessions: 1) Topological solids, with talks given by S. Murakami, B. Yan and O. Yazyev, tackling mostly topological semimetals, in terms of symmetry, topology, and related emergent phenomena; the session also focused on Berry phase related physics and the spin current in antiferromagnetic Weyl semimetals, as well as High-throughput search for novel materials realizing topological electronic phases. 2) Complex magnets, where C. Felser discussed non-collinear spin structures and skyrmions in topologically non-trivial Heusler compounds and T. Jungwirth focused on antiferromagnetic spintronics; 3) Ultra-fast magnetism with talks given by P. Elliott (replacing S. Sharma), focused on ab-initio approaches to all-optical ultrafast switching of magnetic order and by P. Oppeneer, presenting a Theory of ultrafast laser-induced magnetic processes; 4) Two-dimensional spin-orbit solids, where E. Chulkov discussed mainly Quantum spin and anomalous Hall effects in topological insulators (for example prototypical Bi₂Te₃ doped with magnetic impurities) and V. Pardo focused on rutile-based superlattices, with emphasis on spin-orbit effects and non-trivial topological properties; 5) Chiral magnets in which L. Szunyogh addressed chiral spin-textures in nanomagnets, B. Dupé addressed the physics of Skyrmions in 3d-5d metallic multilayers and R. Arita put forward a new order parameter, cluster multipole, to characterize anomalous Hall effects in antiferromagnets; 6) Correlation, cooperative phenomena and SOC, where J. van den Brink addressed the “effective J-half” physics in iridates and potential Kitaev spin-liquids, as recently discussed in RuCl₃, K. Yamauchi focused on the coupling between ferroelectricity, spin texture, and topological properties in transition-metal oxides, with emphasis on novel multiferroics and N. Kioussis addressed topological effects in chalcogenides-based alloys and heterostructures. 7) Theory of spin-orbit torque, where M. Stiles addressed spin-orbit torques from different modeling points of view (ranging from classical to semiclassical to first-principles approaches), F. Freimuth described the formalism developed to treat Dzyaloshinskii-Moriya interaction and spin-orbit torques in noncollinear magnets from first-principles density-functional theory and B. Nikolic discussed spectral functions and spin textures in magnetic heterostructures to get hints on the physics related to spin-orbit torque; 8) Dynamical spin excitations were addressed by M. dos Santos Dias focusing on time-dependent density functional theory simulations to treat Dynamical spin excitations in magnetic nanostructures and by A. Bergman to discuss the theoretical formalism (within atomistic spin dynamics) and results for magnetic excitations in low-dimensional and complex systems; 9) round table on (little understood) Orbital magnetism, magnetoelectric response and related “Berry-ology” (with large and active participation by the audience) and 10) Theory of spin transport, where J. Zelezny (replacing S. Sanvito) discussed calculation of spin-Hall conductivity in topological materials, P. Kelly focused on spin transport from fully relativistic scattering theory at finite temperatures and A. Mook presented his activity on the development of the formalism, related implementation and simulations in the field of Spin and heat transport by magnons.

Community needs

In terms of computational infrastructures, we remark that the community has recently invested sizeable efforts - and plans to invest in the future - on the development of first-principles codes to implement recently proposed spin-orbit-related features (i.e. to evaluate Dzyaloshinskii-Moriya interaction, various Hall conductivities, topological invariants, magnetic excitations, etc). In terms of HPC resources, some of the simulations (presented at or stimulated by the conference, such as for example the evaluation of symmetric and anti-symmetric exchange coupling constants within perturbation theory) certainly require the availability of massive grants at HPC supercomputing centers. The “ab-initio Spin-orbitronics” community is overall well connected to other closely-related communities, such as experimentalists and various theoreticians, ranging from those working on many-body to phenomenological Hamiltonian-modelling to micromagnetic simulations. However, the field is so fastly growing that concerted interdisciplinary efforts need to be carried out at all levels; to this end, a better integration with close communities has definitely to be encouraged, including the interface to industrial partners possibly interested in spin-orbitronics.

Funding

Typical funding channels in “Ab-initio spin-orbitronics” are available at the European level in the H2020 program (in closer detail, within open-FET – Future and Emerging Technology - calls and within the European Research Council, ERC). We note that several FET and ERC grants were recently awarded in the “spin-orbitronics” field. At the national scale the situation is quite heterogeneous. We however note that especially in Germany, several initiatives adequately took into account topics of interest for the community, such as topological matter, spintronics, spin-orbitronics. Many possible collaborations and perspectives for joint applications in the upcoming H2020 calls were discussed among Conference attendees.

Will these developments bring societal benefits?

Information and communication technology in charge-based electronics is rapidly approaching the limits in terms of capacity, speed, as well as energy consumption. Novel paradigms based on spin, topology and electronic correlations (all topics largely discussed at the conference) are appearing as future ingredients to efficiently store and process information. Further promising directions are represented by possible energy efficiency achieved by exploiting multifunctional materials (such as multiferroics) and by the integration of memristive functions based on metal oxides and chalcogenides (i.e. “spin-orbit-active” materials) in view of applications as memory and logic devices and neuromorphic computing. In this framework, the spin-orbitronics field is relatively young and efforts need to be put in the coming years on the understanding of basic physics and related microscopic mechanisms underlying exotic phenomena occurring in spin-orbit materials. To this end, first-principles simulations, in parallel with developments of theoretical formalisms (especially in subfields such as spin-dynamics, spin-transport, magnetoelectric responses, etc) and their related implementation in existing DFT codes, appear of paramount importance.

Conference Program

Monday , 25	13:00	Registration	
	14:00	Welcome	
	14:10	Stuart Parkin	<i>Plenary talk on spin-orbitronics</i>
	15:00	Shuichi Murakami	<i>Symmetry, topology, and emergent phenomena in topological semimetals</i>
	16:00	Coffee Break	
	16:30	Binghai Yan	<i>The Berry phase and the spin current in afm Weyl semimetals</i>
	17:30	Oleg Yazyev	<i>Computational search for novel materials realizing topological electronic phases</i>
	18:30	Poster Session	
	20:30		
Tuesday , 26	9:00	Claudia Felser	<i>Topology, non-collinear spin structures and skyrmions in Heusler compounds</i>
	10:00	Tomas Jungwirth	<i>Thz electrical writing speed in an antiferromagnetic memory</i>
	11:00	Coffee Break	
	11:30	Sangeeta Sharma	<i>All optical ultrafast switching of magnetic order: an ab-initio study</i>
	12:30	Peter Oppeneer	<i>Theory of ultrafast laser-induced magnetic processes</i>
	13:30	Lunch	
	15:00	Eugene Chulkov	<i>Quantum spin and anomalous hall effects in topological insulators: physics and materials science aspects</i>
	16:00	Tim O. Wehling	<i>Magnetism and electron correlations in atoms at surfaces: orbital physics and Hund's rule coupling</i>
	17:00	Poster Session	
	19:00		
Wednesday , 27	9:00	Laszlo Szunyogh	<i>Chirality effects in nanomagnets</i>
	10:00	Bertrand Dupé	<i>Skyrmion à la carte</i>
	11:00	Coffee Break	
	11:30	Ryotaro Arita	<i>Cluster multipole theory for anomalous Hall effect in antiferromagnets</i>
	12:30	Lunch	
	14:00	Jeroen van den Brink	<i>Iridates and RuCl3 - from Heisenberg antiferromagnets to potential Kitaev spin-liquids</i>
	15:00	Kunihiko Yamauchi	<i>Interplay between ferroelectricity, spin texture, and topological properties in TMO</i>
	16:00	Coffee Break	
	16:30	Victor Pardo	<i>Spin-orbit effects and non-trivial topological properties in oxide nanostructures</i>
	17:30	Nicholas Kioussis	<i>Search for novel topological Weyl semimetal phases</i>
	18:30		
	20:00	Social Dinner	
	23:00		
Thursday , 28	9:00	Mark Stiles	<i>Spin-orbit torques in a hierarchy of theoretical approaches</i>
	10:00	Frank Freimuth	<i>Spin-orbit torques in noncollinear magnets from first-principles DFT</i>
	11:00	Coffee Break	
	11:30	Branislav Nikolic	<i>Visualizing the anatomy of spin-orbit torques with spectral functions and spin textures around interfaces of magnetic heterostructures</i>
	12:30	Lunch	
	14:00	Manuel dos Santos Dias	<i>Dynamical spin excitations in magnetic nanostructures from TDDFT</i>
	15:00	Anders Bergman	<i>Modelling magnetic excitations in low-dimensional systems and beyond</i>
	16:00	Coffee Break	
	16:30	Round Table	<i>Round table on Orbital magnetism</i>
	18:30		
Friday , 29	9:00	Stefano Sanvito	<i>First principles multi-scale theory for current-driven magnetization dynamics</i>
	10:00	Paul Kelly	<i>Finite temperature spin transport from fully relativistic scattering theory</i>
	11:00	Coffee Break	
	11:30	Alexander Mook	<i>Spin and heat transport by magnons: theory, simulations, and a tad of topology</i>
	12:30	Conclusion	
	12:45		