SCUOLA NORMALE SUPERIORE

RELAZIONE ATTIVITA' ANNUALE DEI PERFEZIONANDI/DOTTORANDI – TERZO/QUARTO ANNO
REPORT ON THE PHD ACTIVITY – THIRD/FORTH YEAR

NOME E COGNOME NAME AND SURNAME	Louis Ponet
DISCIPLINA PHD COURSE	Nanosciences

CORSI FREQUENTATI CON SOSTENIMENTO DI ESAME FINALE ATTENDED COURSES (WITH FINAL EXAM)	VOTAZIONE RIPORTATA MARK	NUMERO DI ORE HOURS

CORSI FREQUENTATI SENZA SOSTENIMENTO DI ESAME FINALE ATTENDED COURSES (ATTENDANCE ONLY)	NUMERO DI ORE HOURS

ALTRE ATTIVITÀ FORMATIVE (SEMINARI, WORKSHOP, SCUOLE ESTIVE, ECC.) – DESCRIZIONE OTHER PHD ORIENTED ACTIVITIES (SEMINARS, WORKSHOPS, SUMMER SCHOOLS, ETC) – DESCRIPTION	NUMERO DI ORE HOURS
MaNEP Winter School: Symmetry and topology: new twists in condensed matter	21
DPG meeting 2019 Regensburg	43
EMRS Nice 2019	30
TRR 80 Summer School 2019: Functionality of Correlated Materials	15.5
Advanced Electronic Structure Methods in Condensed Matter Physics EPFL	19.5
2nd School on Second Principles Density Functional Theory methods and SCALE-UP	24

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ATTIVITÀ DI RICERCA SVOLTA (MAX. 8.000 CARATTERI)*
RESEARCH ACTIVITY (MAX. 8000 CHARACTERS)

This year I started a new project on addressing ultrafst dynamics of spin and charge density waves (SDW, CDW) in chromium. Experiments were performed by Prof. Andrej Singer's group at Cornell University, where x-rays were used for ultrafast excitation and probing of the SDW and CDW. The x-ray pulses heat up (and potentially melt) the SDW which in turn shifts the potential for the associated strain and CDW such that its amplitude starts oscillating. This oscillation is then monitored by x-ray diffraction. By modulating the delay between pulses, it is possible to cause either constructive or destructive interference with the already present oscillation of the charge density wave, allowing for very fine tuned control. Surprisingly, when the delay between the pump pulses is short, the observed oscillations are lower than for pulses shifted bya period of CDW oscillation. We formulated a model combining Landau theory and heat transfer equations describing the interaction between SDW and CDW order parameters, and their dynamics. The temperature of the SDW is described by a two temperature model, where heat is exchanged between the SDW and a phonon bath, and the pump pulses supply heat to the SDW. The first order character of the SDW phase transition is also accounted for.
The parameters of the model were then fitted to the experimental data, leading to a very good agreement. Results show that reduced oscillation amplitude, observed for short delays between pumps, is related to SDW melting transition. Using the model, we are able to generate a train of pulsesthat drives CDW oscillations with the envelope of a chosen form. This ability to control the DW has not yet been tested experimentally. We are currently in the final stages of preparing the paper for submission.

I continued work on soft domain wall-localized phonons, in order to describe mechanial softening that is observed by Prof. Gustau Catalan's group near 180 degree ferroelectric domain walls in BaTiO3. We simulate the behavior of the wall and domain with and without a tip with the finite element method, which turned out to be more involved than we expected at the start of the project. We managed to corraborate our results with another theoretical group and reproduce the experimental observations well. We're also in the last stages of writing this paper.

I also assisted in finalizing a paper on a related project about the theoretical explanation of an anomalous activation of phonon modes in BiFeO3 R71 domain walls. This was experimentally observed by Prof. Keji Lai's group at the university of Texas at Austin. One of the related manuscripts is currently under review, and another has been resubmitted after a revision.

In the meantime I also continued the work on calculating parameters of magnetic Hamiltonians for materials with either high spin-orbit coupling, or noncolinear magnetism. In these materials the well-understood Heisenberg model doesn't describe the magnetic structures, and anisotropic

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interactions are important. This is because either spin is not a good quantum number for the on-site Hamiltonian (in the high spin-orbit coupled case) and the magnetism is caused by both spin and orbital angular momentum, or simply because the situation of noncolinear spins was not included in previous derivations/implementations. We are focusing on Sr_2IrO_4, $NaIrO_3$, Mn_3Sn but technical limitations of DFT codes still need to be overcome and we therefore haven't been able to fully test our theory and implementation, and so far there are no real results.

I have given a talk on our progress with calculating the exchanges in the DPG Regensburg meeting.

*se si intende sottoporre una relazione di ricerca più estesa, utilizzare il campo per una descrizione sintetica e allegare il documento in formato .pdf

If you are going to submit a longer report, please fill the box with a synthetic abstract and attach a document in pdf format

EVENTUALI PUBBLICAZIONI **PUBLICATIONS (IF AVAILABLE)**
First-principles theory of giant Rashba-like spin splitting in bulk GeTe - Phys. Rev. B 98, 174102

NOME DEL RELATORE **THESIS ADVISOR**
Dr. Sergey Artyukhin

DATA **DATE**	06/10/2019	**FIRMA** **SIGNATURE**	[signature]