Dynamics In Functional Materials

12th-14th Feb 2020

Goa, India

Organizers: **Biplab Sanyal**, Uppsala University, Sweden & **Bhalchandra Pujari**, Savitribai Phule Pune University, India

The conference is organized as a part of Swedish Research Links project granted by Swedish Research Council

Day 1: 12th Feb 2020

08:30 - 09:15	Registrations and welcome	
09:15 - 10:15	Keynote lecture	Hermann Dürr
10:15 - 10:45	Coffee break	
10:45 - 11:45	Keynote lecture	Dilip Kanhere
11:45 - 12:30	Invited talk	Pedro Melo
12:30 - 14:00	Lunch break	
14:00 - 14:45	Invited talk	Oscar Grånäs
14:45 - 15:30	Invited talk	Pralay Santra
15:30 - 16:00	Coffee break	
16:00 - 16:45	Invited talk	Santosh Kumar
16:45 - 17:05	Contributed talk	Raquel Esteban
17.05 - 17.25	Contributed talk	Xin Chen
17.30-18.30	Poster session	

Day 2: 13th Feb 2020

08:30 - 09:30	Keynote lecture	Olof Karis
09:30 – 10:30	Keynote lecture	D. D. Sarma
10:30 - 11:00	Coffee break	
11:00 - 11:45	Invited talk	Anna Delin
11:45 - 12:30	Invited talk	Mukul Kabir
12:30 - 14:00	Lunch break	
14:00 - 14:45	Invited talk	Saurabh Ghosh
14:45 - 15:30	Invited talk	Sudipta Kanungo
15:30 - 16:00	Coffee break	
16:00 - 16:45	Invited talk	Madhura Marathe
16:45 - 17:05	Contributed talk	Alexey Lukoyanov
17.05-17.25	Contributed talk	Elena Shreder
17.25 – 17.45	Contributed talk	Duo Wang

19.30: Conference dinner

Day 3: 14th Feb 2020

08:30 - 09:15	Invited talk	Subhradip Ghosh
09:15- 10:00	Invited talk	Pooja Goddard
10:00 - 10:30	Coffee break	
10:30 - 11:15	Invited talk	Kartick Tarafder
11:15 - 12:00	General discussions & concluding remarks	
12:00 - 14.00	Lunch & departure	

Tracking the non-equilibrium energy flow between

electron, spin and lattice degrees of freedom

Hermann Dürr
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The idea to probe, change and control functional materials properties with the help of light has long intrigued researchers in materials science. Using femtosecond laser pulses it is now possible to control the magnetic order or even enhance superconductivity. Femtosecond laser excitation of solid-state systems creates out-of-equilibrium hot electrons that cool down by transferring their energy to other degrees of freedom and ultimately to lattice vibrations of the solid. The understanding of this strongly non-equilibrium dynamics in solids is still very limited, in spite of its emerging importance from a fundamental and applied science viewpoint. The three-temperature model, commonly used for magnetic metals, assumes that the electronic, spin and lattice subsystems are each in separate equilibrium at all times and reach global equilibrium by exchanging heat. The equilibrium concept of “temperature” is so powerful that is is often ignored that it takes time before non-equilibrium dynamics can be described by it. In this lecture I will give an overview how modern ultrafast spectroscopy and scattering techniques allow us to determine in a momentum-resolved way the electron, spin and lattice excitations in the laser-heated state. These results demonstrate that we need to view non-equilibrium dynamics by its associated flow of energy between the various degrees of freedom.

Time Dependent Density Functional theory : Basics

Dilip Kanhere
Savitribai Phule Pune University, India

In the first part I plan to present an overview of basic time dependent density functional theory. It includes Runge Gross theorem, causality problem, linear response, direct evolution and a few important applications.

In the second part I plan to give flavours of non-adiabatic dynamics.

Ultrafast dynamics in transition metal dichalcogenides

Pedro Melo
University of Leige, Belgium

The emergence of ultrafast pump-and-probe techniques has brought to light an immense amount of information on the dynamics of materials after excitation by a laser field. When these techniques are used on transition metal dichalcogenides (TMDs), we also have access to a coupling between the spin and valley degrees of freedom. This fascinating effect allows us to use circularly polarised light to select in which valley to create a population of excited carriers. If the depolarisation time scale after excitation is large enough, this pseudospin can open the door to new devices which use valleytronics. However, to understand the photo-generation and relaxation mechanisms we need an accurate description of the interactions of coupled out-of-equilibrium dynamics of photons, phonons, and electrons. Here we will present an ab-initio method to study the ultrafast pump and probe experiments and how we deal with the different particles involved in the relaxation processes. We will show how the electron-phonon interaction changes the optical properties of TMDs and provide insight to the microscopic dynamics happening in these materials in pump-and-probe experiments.

Towards a first-principles framework for correlated materials out of equilibrium

- Non-adiabatic dynamics with time-dependent density-functional theory

Oscar Grånäs

Uppsala University, Sweden

The description of intrinsically quantum mechanical phenomena is a great challenge for computational science. A particular difficulty is the first-principles description of light induced ultrafast phenomena where there is a strong coupling between electronic, magnetic and ionic degrees of freedom. In this talk I give a brief overview of time-dependent density-functional theory and how it can be used to tackle these systems. I outline the main approximations used in the current state of the art, as well as a route to address shortcomings.

Further, I present two examples where time-dependent density functional theory is used in conjunction with recent experimental techniques to study two prototype correlated systems driven out of equilibrium.

Charge transfer and ion movements in semiconductor nanocrystals

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Manipulation of energy and electron transfer processes in light-harvesting assemblies is an important criterion to make an efficient solar cell. Of particular interest is the quantum dot sensitized solar cells as they offer bandgap tunability through size and composition, hot electron injection etc. In the first part of my talk, I will discuss the electron transfer processes in doped and undoped quantum dot sensitized solar cells and how these understandings have helped us in understanding the luminescence-based gas sensors using quantum dots.

In the second part of the talk, I will be discussing the anion exchange of pre-synthesized cesium lead halide nanocrystals - which has a very low activation energy of 0.75 ± 0.05 eV. The passivating ligands, which are in dynamic equilibrium with the nanocrystals and the solution, play an important role in such ion exchanges.

References:

1. Santra PK, Kamat P V. Mn-doped quantum dot sensitized solar cells: A strategy to boost efficiency over 5%. *J Am Chem Soc*. 2012;134:2508-2511. doi:10.1021/ja211224s
2. Santra PK, Chen YS. Role of Mn^{2+} in doped quantum dot solar cell. *Electrochim Acta*. 2014;146:654-658. doi:10.1016/j.electacta.2014.08.145
3. Devaiah Chonamada T, Sharma B, Nagesh J, et al. Origin of Luminescence-Based Detection of Metal Ions by Mn–Doped ZnS Quantum Dots. *ChemistrySelect*. 2019;4:13551-13557. doi:10.1002/slct.201903769
4. Haque Anamul, Devaiah Chonamada T, Dey Arka B, Santra PK. Visualization of Halide Ion Migration and the Kinetics of Interparticle Mixing of $CsPbBr_3$ and $CsPbI_3$ Nanocubes, *Unpublished* 2020

2D Materials: An Intriguing Quantum-photonic Platform

Santosh Kumar
IIT Goa

Olof Karis
Uppsala University, Sweden

Time-resolved investigations of opto-electronic materials in the sub-ps regime

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Self-absorption has been a major impediment to utilizing brilliant and tunable photoluminescence from semiconductor nanocrystals, as it reduces drastically the quantum efficiency at any reasonable optical density. In this context, defect emissions are interesting because of their Stokes shifts that make them impervious to self-absorption, but this comes often at the cost of the quantum efficiency and the tunability. We have been addressing these issues for many years and have overcome these challenges in carefully designed systems.[1-4] Ultrafast spectroscopic studies allow us to probe the origin of the high quantum efficiencies in such systems and I shall discuss two such systems in this talk.

If time permits, I shall also discuss a fundamental issue related to the spectacular photovoltaic properties observed in hybrid perovskite halides and address the intriguing possibility of an excited state polarization of the material due to the presence of dynamical dipoles in the ground state.[5]

These three examples illustrate different time-resolved techniques that we employ to understand properties of materials within our group.

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3. Abhijit Hazarika et al., unpublished results
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5. Sharada Govinda et al., J. Phys. Chem. Lett. 2017, **8**, 4113.

Spin dynamics and spin-heat interaction

Anna Delin
KTH, Sweden

Temperature and temperature gradients have profound effects on the magnetic and spin-dynamic properties of materials. The phonon-magnon coupling directly affects a number of dynamical processes such as demagnetization processes, thermal conductivity, magnetoacoustics, and the spin-Seebeck effect. The interaction between spin and lattice motion is also central for phenomena observed in magnetoelectric and in multiferroic materials, magnetocaloric materials, skutterudites, and antiferromagnetic insulator materials for spintronic devices.

In this talk, I will present our recently developed method for explicit spin-lattice simulations, based on a spin-lattice Hamiltonian, where the bilinear magnetic term is expanded up to second order in displacement. If time permits, I will also present our work on skyrmion stability at finite temperature and how temperature gradients may give rise to surprising magnetic phenomena such as a spincaloritronic diode effect, or domain wall motion in the absence of both spin current and magnetic field.

Two-dimensional phosphorene: The new wonder material?

Mukul Kabir
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Phosphorene, a monolayer of black phosphorus with anisotropic mechanical, electronic and optical properties, has become the second most sought-after two-dimensional material after graphene. This elemental 2D material, with a *right* semiconducting gap and high carrier mobility, may lead to future electronic applications. Further, it has attracted enormous attention to investigate many-body physics. However, the biggest challenge lies in its stability, leading to mechanical and chemical degradations. In this talk, we will review our group's effort in phosphorene on the various topics in degradation, magnetism, Kondo state, optics and exciton.

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Saurabh Ghosh
SRM University, India

Tale of exotic magnetic phase transition in Os based double-perovskites: microscopic insights from first principles calculations

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Transition metal oxides (TMO) are an evergreen filed of research from the magnetism point of view as this class exhibits most variety; such as AFM, Ferri, canted-AFM, spin-glass, spin-liquid, spin-gap phase, spin-state transitions, quantum phase transition etc. 5d TMOs, where correlation, spin-orbit coupling and crystal filed splitting are competing, forms a new emerging field of research with huge promise for realizing different novel phases such as toplological insulator, quenched magnetism, anisotropy etc. These various novel phenomena arise due to interplay of charge, lattice, orbital and spin degrees of freedom, which are governed by the "electrons". Therefore, understanding of underlying electronic structure from *ab-initio* perspective is indispensable for understanding the mechanism of the properties and engineering the properties.

This presentation is devoted to the study of microscopic origin of exciting and intriguing low temperature magnetic behaviour of complex Sr_2BOsO_6 (B=Y, In, Sc) double-perovskite materials, employing density functional theory based first principles electronic structure calculations. All these three compounds only Os^{+5} ($5d^3$) is magnetically active site and other transition metal sites (Y/In/Sc) is magnetically inactive either completely filled (d^{10}) or empty (d^0) d states. Although these three compounds are iso-electronic, isovalent and iso-structural, their antiferromagnetic transition temperatures are widely different from 92K to 27K. Our electronic structure calculations and magnetic exchange interaction calculation revealed this apparently counterintuitive trend of transition temperature. Our calculations demonstrate the active role of the nonmagnetic transition metals, whether it is d^0 or d^{10}, dictates magnetic transition temperatures in terms strong hybridization between nonmagnetic (B) sites with the magnetic Os site.

References

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2. Sudipta Kanungo*, Binghai Yan*, Martin Jansen, and Claudia Felser. **Phys. Rev. B 89, 214414 (2014).**

3. B. Yan, A. Paul, S. Kanungo, M. Reehuis, A. Hoser, D. Többens, W. Schnelle, R. Williams, T. Lancaster, F. Xiao, J. Möller, S. Blundell, W. Hayes, C. Felser, and M. Jansen. **Phys. Rev. Lett. 112, 147202 (2014).**

First-principles simulations of Electrocaloric effect in bulk $BaTiO_3$

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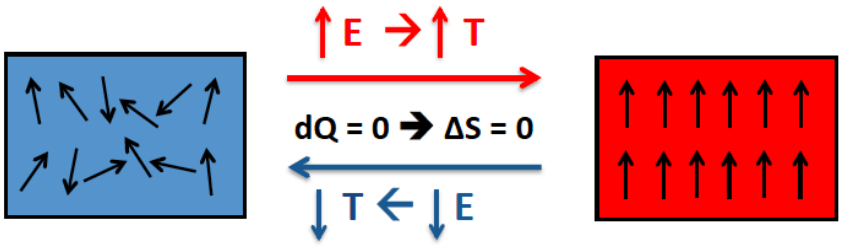
The electrocaloric (EC) effect describes a change in temperature (or entropy) of a material under adiabatic (or isothermal) application of an electric field. The application of field aligns the dipoles resulting in the increase of system temperature when there is no heat exchange with surroundings, and vice versa removal of field reduces the temperature (see figure). This effect is very attractive for potential applications in solid-state cooling devices. The largest effect is observed in ferroelectric (FE) materials near the paraelectric-ferroelectric transition.



In this talk, I would explain the EC effect and discuss some of our results performed using molecular dynamics simulations of a first-principles based effective Hamiltonian. We use bulk barium titanate as our model system which is a well-studied perovskite ferroelectric material. We have studied how to tune the response to get a large temperature change by applying an epitaxial strain [1]. Further, I will discuss an inverse EC effect, that is, an increase in the system temperature on field removal observed at FE-FE transitions in $BaTiO_3$ and how we understand it using the generalized Clausius-Clapeyron equation [2,3].

References
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DFT calculation of quantum capacitance in MXene based supercapacitor electrodes

Subhradip Ghosh
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2D materials based supercapacitors have drawn considerable attention in recent times. The available large surface area of 2D materials have made them useful for storage of large amount of charges. Recently discovered 2D MXenes have shown substantial potential as supercapacitor electrode materials. Quantum capacitance is one of the quantities relevant for the supercapacitative performance. In this work, we present results on quantum capacitances of a number of MXenes, in pristine and in functionalized forms. We analyse the results by comparing their electronic structres.

CdTe - A Thin Film Solar Cell Material - a DFT viewpoint

Pooja Goddard
Loughborough University, UK

Cadmium telluride is the leading technology for thin-film solar cells. As deposited, CdTe films contain a very high concentration of stacking faults and exhibit poor photovoltaic efficiency. An extra annealing treatment with CdCl2 is required to produce high efficiency cells. Although the precise mechanism for this performance increase is unknown, the concentration of stacking faults is greatly reduced in treated cells.
This work uses high accuracy density functional theory calculations to investigate the role of stacking faults in CdTe. All experimentally observed faults have been investigated and will be discussed in detail in relation to band gaps and structural defects. Further to this, Se doping has been known to increase efficiency through band gap grading. We report the effect of Se doping on the band gap and the optical transition probability. Finally, The talk will discuss some computational modelling of Ar bubbles observed in CdTe thin films that have been sputtered. Here comparison between Ar and Xe will discussed as will the mechanisms of the bubble formation.

Transition Metal Quinonoids for Spintronic applications: Insight from First principle calculations

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Quinonoids are promising molecules, well known for their applications in physical chemistry, color chemistry and drag designing . These molecules and their derivatives are high pH-selective and pH-sensitive. Their presence in organic thin films significantly enhances the charge carrier concentrations. As a result, highly conductive interface can be formed by adsorbing these molecule and their derivatives on metal/semi-conducting surfaces . Therefore considering quinonoids and their derivatives as active centers, one can take part in developing new functional materials. In addition, metal-organic quinonoid molecules are potential building blocks in coordination polymers as well as materials useful for catalysis, surface chemistry, and molecular spintronics. In this presentation I shall discuss electronic and magnetic properties of few recently synthesized Transition Metal-quinonoid complexes and their interactions with magnetic substrates. Discussion will be focus on mono and dinuclear transition metal-quinonoid complexes, which shows interesting magnetic and opto-electronic behavior. A recent observation of an unexpected antiferromagnetic coupling of the molecule to the ferromagnetic Co(001) substrate will also be discussed.

References:

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Contributed talks

Raquel Esteban, Uppsala University, Sweden
Tailoring the opto-electronic response of graphene nanoflakes by size and shape optimization

Xin Chen, Uppsala University, Sweden
Two-dimensional square-A_2B (A=Cu, Ag, Au, and B=S, Se): Auxetic semiconductors with high carrier mobilities and unusually low lattice thermal conductivities

Alexey Lukoyanov, M.N.M. Institute of Metal Physics, Russia
Effect of structural disorder on the electronic structure and physical properties of the Heusler Co_2CrAl and Co_2NiAl alloys

Elena Shreder, M.N.M. Institute of Metal Physics, Russia
Composition dependence of Optical properties of Mn2-xFe1+xAl Heusler alloys

Duo Wang, Uppsala University, Sweden
First principles calculations and Monte Carlo simulations of half-metallic quadruple perovskite $ACu_3Fe_2Re_2O_{12}$ (A=Ca, Ba, Sr, Pb, Y, La, Sc)

Posters

Reshma Rajeev L, SRM University
Structural, electronic and magnetic properties of Mn/Fe doped and (Mn, Fe) codoped $Zn_{12}O_{12}$ Dimer

Chandan Singh, IISER, Pune
Superconducting spin-valve in van der Waals heterostructure

Deepak Kumar Roy, IISER, Pune
Electron correlation and magnetic structure in perovskite oxides

Satyananda Chabungbam, IISER, Turupati
Strain tunable magnetism in hetero-bilayers of transition metal trichalcogenides

Monirul Shaikh, SRM University
Defect induced ferromagnetism in two dimensional $Cr(COOH)_3$ metal-organic frameworks

Anup Shrivastsava, IIIT Allahabad
Investigations of Optoelectronic behavior Sb-hBN bilayer

Sanjay Kumar Singh, S. D. college, Punjab
Phase Transition Properties of NdX (X = P, As) : A Full-Potential Study

Mohammad Ubaid, Jami Milia Islamia University
Electronic Properties of Blue Phosphorene/TiS_2 vdW Heterostrucure