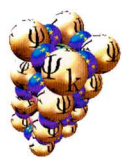




The Abdus Salam  
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## 18th International Workshop on *Computational Physics and Materials Science: Total Energy and Force Methods* January 12-14, 2017 Miramare, Trieste, Italy

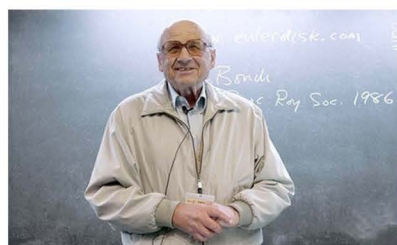
This Workshop is held traditionally in Trieste every two years, since 1987. Following the tradition of the previous meetings, it will be devoted to recent advances in computational condensed matter physics and materials science, based on realistic calculations of the electronic structure of complex systems.

The activity will be held at the International Centre for Theoretical Physics (ICTP), Trieste, Italy from 12 to 14 January 2017 with the co-sponsorship of Psi-k, SISSA, Consortium for Physics of Trieste, MaX EU Centre of Excellence for HPC applications, the European Cooperation in Science and Technology (COST) and the EUSpec Action "Modern Tools for Spectroscopy on Advanced Materials".

As in previous events of this series, the Workshop will consist of invited talks and contributed poster sessions, with ample space devoted to discussion.

Topics will span a broad range, including, among others:

- Spectroscopy
- Strong electronic correlations
- Electron-phonon coupling
- Superconductivity
- Novel functionals
- Transport
- Advanced Materials
- Materials Discovery



A special session will be held in memory of **Walter Kohn**, admired mentor and role model for many students and colleagues, who was awarded the [Nobel Prize in Chemistry](#) for his development of the density functional theory. The session will include the Award ceremony for the "Walter Kohn prize for quantum mechanical material modeling" (<https://www.ictp.it/about-ictp/prizes-awards/walter-kohn-prize.aspx>), co-funded by ICTP and the Quantum ESPRESSO Foundation.

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12/01/2017 - 14/01/2017

Trieste, Italy

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# **PROGRAMME**



# 18th International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods | (smr 3101)

Thursday, 12 January 2017

08:30 - 09:10

Location: Leonardo Building - Budinich Lecture Hall

08:30 **Registration and Administrative Formalities: Upon arrival, all Faculty(Directors, Speakers) & those in outside Hotels ONLY, are kindly requested to complete registration formalities from 8:30 am and throughout the day/week at the Secretariat, Lobby, Leonardo Building (venue). [Participants are now registered, upon check-in at the ICTP Guesthouses.] After you have Registered (Faculty and Participants whose expenses are covered by the ICTP): Administrative Formalities (daily living allowances/travel reimbursements, bank transactions, etc.) at the E. Fermi Building [just above the Leonardo Da Vinci Bldg.], Operations' Unit [Mondays, Tuesdays & Fridays ONLY, 8:30 - 12:00 & 1:30 - 2:30] , Tuesday - Friday 13.00-15.00; UNICREDIT Bank, Mondays & Fridays ONLY, 8:30 - 1:20 & 2:30 - 4:00. 30'** (Leonardo Building - Lobby)

09:00 **Welcome & Introduction: Directors 10'**

Speaker: S. Narasimhan, M. Peressi, L Reining

09:10 - 10:15

Session: Ferroelectricity

09:10 **Introduction to the session 5'**

09:15 **Charge-order-driven ferroelectricity in perovskite superlattices from first principles 30'**

Speaker: K. Rabe (Rutgers The State University of New Jersey)

09:45 **Interplay between Ferroelectricity and Rashba effects 30'**

Speaker: S. Picozzi (CNR-SPIN Chieti)

10:15 - 11:10

Lecture in Honor of Walter Kohn

10:15 **Walter Kohn: The Science and the Man 30'**

Speaker: E.K.U. Gross (Max Planck Institute of Microstructure Physics, Halle)

10:45 **Coffee Break 25'** (Leonardo Building - Lobby)

11:10 - 14:20

Session: Charge and Spin Correlations

11:10 **Introduction to the session 5'**

11:15 **Exchange-Correlation functionals inspired to the exact strong-coupling limit of density functional theory 30'**

Speaker: P. Gori-Giorgi (Vrije Universiteit Amsterdam)

11:45 **Electronic Structure and Lattice Stability of Correlated Electron Materials 30'**

Speaker: I. Leonov (Institute of Physics, University of Augsburg)

12:15 **Spin caloritronics and spin dynamics in low-dimensional systems 30'**

Speaker: A. Delin (Electrum, Sweden)

12:45 **Lunch Break 1h35'** (Leonardo Building - Cafeteria)

- 14:20 - 16:25 Session: Electronic excitations
- 14:20 **Introduction to the session 5'**
- 14:25 **Exciton binding and instabilities in quasi-1d Carbon based systems 30'**  
Speaker: E. Molinari (Univ. Modena e Reggio Emilia, and CNR-NANO, Modena, Italy)
- 14:55 **Modeling Light-Matter interactions: Quantum Electrodynamics (QED) Chemistry and Materials within TDDFT 30'**  
Speaker: A. Rubio (Max Planck Institute for the Structure & Dynamics of Matter, Hamburg)
- 15:25 **Coupled-cluster theory for condensed-phase spectroscopy 30'**  
Speaker: T. Berkelbach (the University of Chicago, Dept. of Chemistry)
- 15:55 **Coffee Break 30'** (Leonardo Building - Lobby)
- 16:25 - 17:30 Session: Optical properties
- 16:25 **Introduction to the session 5'**
- 16:30 **Excited-State Phenomena in Organic Materials and at Interfaces from First Principles 30'**  
Speaker: J. B. Neaton (Molecular Foundry, Lawrence Berkeley National Laboratory)
- 17:00 **A High-Throughput Computational Search for New Transparent Conducting Oxides and New Thermoelectrics 30'**  
Speaker: G. Rignanese (Institut de la matière Condensée et des Nanosciences, Louvain La Neuve)
- 18:00 - 20:00 POSTER SESSION 1: (If needed posters can be printed in an A0-format, at our in-house printshop.) At Adriatico Guest House: outside KLH, 26 wall-mounted boards, mts.1.00 (width) x 2.00 (height) for a total of 26.00 sq.mts. + 4 mobile boards of 4 faces each, size of each face: mts 1,20 (width) x1,90 (height); total 16 faces for 36.48 sq. mts.  
Location: Adriatico Guest House - (Lower Level 1)
- 18:00 **A Reception will be offered during the poster session. 2h0'**

## Friday, 13 January 2017

- 09:00 - 11:05 SPECIAL SESSION in Honour of Walter Kohn  
Location: Leonardo Building - Budinich Lecture Hall
- 09:00 **Introduction to the session 1h0'**
- 10:00 **Walter Kohn Prize Ceremony and Walter Kohn Award Lecture: "Atomistic Structure Prediction via Swarm Intelligence Algorithms 35'**  
Speaker: Yanming Ma (State Key Lab of Superhard Materials, Jilin University, Changchun)
- 10:35 **Coffee Break 30'** (Leonardo Building - Lobby)
- 11:05 - 14:00 Session: Topological and emergent properties
- 11:05 **Introduction to the session 5'**
- 11:10 **Topological Electronic States and Materials 30'**  
Speaker: Z. Fang (Institute of Physics, CAS)
- 11:40 **Emergent Behavior in Thermal Transport 30'**  
Speaker: A. Cepellotti (THEOS, MARVEL, Univ. Berkely)
- 12:10 **Lunch Break 1h50'** (Leonardo Building - Cafeteria)
- 14:00 - 16:05 Session: Sampling methods: developments and applications
- 14:00 **Introduction to the session 5'**
- 14:05 **Atomistic mechanisms and kinetics during phase transformations in metals 30'**  
Speaker: J. Rogal (Interdisciplinary Centre for Advanced Materials Simulation, ICAMS, Bochum)
- 14:35 **Improving the scalings of Quantum Monte Carlo methods with multi-determinant expansions 30'**  
Speaker: R. Assaraf (Université P. et M. Curie, D. Chemistry, Paris)
- 15:05 **Entropy as a collective variable 30'**  
Speaker: M. Parrinello (ETH Zurich & Università della Svizzera Italiana, Lugano)
- 15:35 **Coffee Break 30'** (Leonardo Building - Lobby)
- 16:05 - 17:40 Session: Temperature and phonon effects, thermal transport
- 16:05 **Introduction to the session 5'**
- 16:10 **Car and Parrinello meet Green and Kubo: simulating atomic heat transport from equilibrium ab initio molecular dynamics 30'**



Speaker: S. Baroni (SISSA, Trieste)

16:40 **Non-locality in lattice thermal conductivity** 30'

Speaker: P. Allen (Stony Brook University, New York)

17:10 **One-shot calculation of temperature-dependent optical spectra and phonon-induced band-gap renormalization** 30'

Speaker: F. Giustino (Department of Materials, University of Oxford)

18:00 - 20:00

POSTER SESSION 2: (If needed posters can be printed in an A0-format, at our in-house printshop.) At Adriatico Guest House: outside KLH, 26 wall-mounted boards, mts.1.00 (width) x 2.00 (height) for a total of 26.00 sq.mts. + 4 mobile boards of 4 faces each, size of each face: mts 1,20 (width) x1,90 (height); total 16 faces for 36.48 sq. mts.

Location: Adriatico Guest House - (Lower Level 1)

18:00 **A Reception will be offered during the poster session.** 2h0'

Saturday, 14 January 2017

09:00 - 11:35

Session: Functionals and efficient approaches

Location: Leonardo Building - Budinich Lecture Hall

09:00 **Introduction to the session** 5'

09:05 **Advances in semi-empirical density functionals for molecules and materials** 30'

Speaker: M. Head-Gordon (Dept. of Chemistry, Univ. of California, Berkeley and Chemical Sciences Division, Lawrence Berkeley National Laboratory)

09:35 **Electron correlation from the adiabatic-connection-fluctuation-dissipation-theorem approach for a multireference wavefunction** 30'

Speaker: K. Pernal (Technical University of Lodz Institute of Physics)

10:05 **Strongly Constrained and Appropriately Normed (SCAN) Semilocal Density Functional: Accurate and Efficient for Structures and Energies of Diversely-Bonded Materials** 30'

Speaker: J. Sun (Department of Physics The University of Texas at El Paso)

10:35 **Large Scale Many-Body Perturbation Theory Calculations: Methodological Developments, Data Collections, Validation and Applications** 30'

Speaker: M. Govoni (Materials Science Division Argonne National Laboratory)

11:05 **Concluding Remarks** 30'

**ABSTRACTS**  
**OF**  
**INVITED TALKS**

**(in talk order)**



**Title: Charge-order-driven ferroelectricity in perovskite superlattices  
from first principles**

**K. Rabe**

Department of Physics and Astronomy  
Rutgers The State University of New Jersey  
USA

*Abstract:*

The application of first-principles methods to the systematic study of families of materials opens up new avenues to the theoretical design of materials with targeted functional properties. In this talk, I will discuss recent work on the systematic study of selected families of perovskite superlattices, including structure determination and investigation of charge disproportionation and charge ordering, magnetic ordering and Jahn-Teller distortions. The resulting identification of the 1:1 LaVO<sub>3</sub>/SrVO<sub>3</sub> superlattice as a candidate charge-order-driven ferroelectric, and novel aspects of the electric polarization in this electronic ferroelectric, will be presented and discussed.

# Interplay between Ferroelectricity and Rashba effects

Silvia Picozzi,

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c/o Univ. "G. D'Annunzio" Chieti-Pescara, 66100 Chieti, Italy,  
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Keywords: Ferroelectricity, spin-orbit coupling, Rashba effects

## Abstract

The discovery of novel properties, effects or microscopic mechanisms in modern materials science is often driven by the quest for the coexistence and/or coupling of several functional properties into a single compound. Within this framework, by exploiting the interplay between spin and dipolar degrees of freedom via spin-orbit coupling in ferroelectric semiconductors, I will focus on the tight link between  $k$ -dependent spin-splitting in the electronic structure, spin-texture and electric polarization. Based on density functional simulations, I will show our theoretical predictions of a giant Rashba spin-splitting in "bulk" GeTe<sup>1</sup>, prototype of novel multifunctional materials - labeled as Ferro-Electric Rashba Semi-Conductors (FERSC)<sup>2</sup> - where the chirality of the spin texture is one-to-one linked to polarization. As the latter can be induced/controlled/switched via an electric field in a non-volatile way, the integration of semiconductor spintronics with ferroelectricity is envisaged. In the second part of the talk, the connection between ferroelectricity and spin-degrees of freedom will be discussed by providing examples from different materials classes (oxides heterostructures,<sup>3</sup> halides perovskites,<sup>4</sup> chalcogenides, etc), all of them showing strong relativistic effects.

## References

<sup>1</sup> D. Di Sante, P. Barone, R. Bertacco and S. Picozzi, *Adv. Mater.* **25**, 509 (2013); M. Liebmann et al, *Adv. Mater.* **28**, 560 (2016)

<sup>2</sup> S. Picozzi, *Front. Physics* **2**, 10 (2014)

<sup>3</sup> K. Yamauchi, P. Barone, T. Shishidou, T. Oguchi and S. Picozzi, *Phys. Rev. Lett.* **115**, 037602 (2015)

<sup>4</sup> A. Stroppa, D. Di Sante, P. Barone, M. Bokdam, G. Kresse, C. Franchini, M.-H. Whangbo, S. Picozzi, *Nature Communications*, **5**, 5900 (2014)



**Title: Exchange-Correlation functionals inspired to the exact strong-coupling limit of density functional theory**

**P. Gori-Giorgi**

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**ABSTRACT:**

The exact strong-coupling limit of density functional theory (DFT) reveals a mathematical structure very different from the one of traditional approximations for the exchange-correlation functionals. Instead of the usual local density, local density gradients, Kohn-Sham orbitals, and related quantities, in this limit we observe the appearance of certain integrals of the density. I will illustrate some approximations that we have proposed inspired to this mathematical structure. These approximations retain some of the non-locality of the exact strong-coupling limit of DFT while being computationally affordable.

## Electronic Structure and Lattice Stability of Correlated Electron Materials

Ivan Leonov

Theoretical Physics III, Center for Electronic Correlations and Magnetism, University of Augsburg, Germany and

Materials Modeling and Development Laboratory, National University of Science and Technology 'MISIS', 119049 Moscow, Russia

The computational studies of the electronic structure and magnetism of strongly correlated electron materials is one of the most challenging theoretical problems. In this talk, I will discuss an application of the novel computational scheme DFT+DMFT to explore the electronic and structural properties of correlated materials [1]. In particular, I will present our recent results for the pressure-induced magnetic collapse and Mott insulator-metal transition in paramagnetic monoxides MnO, FeO, CoO, and NiO. Our calculations reveal that under pressure these materials exhibit a Mott insulator-metal transition (IMT) which is accompanied by a simultaneous collapse of local magnetic moments and lattice volume, implying a complex interplay between chemical bonding and electronic correlations. In addition, I report the electronic properties and phase stability of Fe<sub>2</sub>O<sub>3</sub> near a pressure-induced Mott metal-insulator transition. Our results reveal that upon compression Fe<sub>2</sub>O<sub>3</sub> undergoes a Mott insulator (MI) to site-selective MI phase transition, which is characterized by a collapse of local moments and emergence of metallic state only on half of the Fe sites. In agreement with experiment, it was found that the IMT is accompanied by a structural transformation from corundum to a double perovskite lattice structure. Our results for the electronic state, equilibrium crystal structure, and structural phase stability are in quantitative agreement with experimental data. We find that electronic correlations are important to explain the lattice stability of correlated materials, e.g., in the vicinity of a Mott insulator-metal transition.

[1] I. Leonov et al., Phys. Rev. Lett. 106, 106405 (2011); I. Leonov et al., Phys. Rev. Lett. 115, 106402 (2015); I. Leonov et al., Phys. Rev. B 91, 195115 (2015); I. Leonov et al., Phys. Rev. B 94, 155135 (2016).



Title: *Spin caloritronics and spin dynamics in low-dimensional systems*

**Anna Delin**

Electrum, level 4, Kistagången 16, Kista  
Sweden

**Abstract:**

I will present some recent results involving both atomistic and classical spin dynamics simulations (based on first-principles calculations). These methods can be used to investigate theoretically a range of spin-based phenomena, such as Gilbert damping and spin stiffness. [1,2]

Recently, we have turned some focus toward spin caloritronic phenomena, i.e. the interaction between spin and heat. For example, a thermal gradient can move domain walls via the thermal spin torque. [3]

In the presence of a thermal gradient, we find a rectification of the spin and energy flows in systems of magnetic discs at certain conditions, i.e. a spin caloritronic diode effect. Our model also predicts that energy and magnetization in certain situations may flow between two sources with the same temperature and chemical potential. This latter effect can be compared to the well-known dc Josephson effect in superconductors. [4,5]

**References:**

[1] Philipp Dürrenfeld, Felicitas Gerhard, Jonathan Chico, Randy K Dumas, Mojtaba Ranjbar, Anders Bergman, Lars Bergqvist, Anna Delin, Charles Gould, Laurens W Molenkamp, Johan Åkerman (2015). Tunable damping, saturation magnetization, and exchange stiffness of half-Heusler NiMnSb thin films, Phys. Rev. B 92, 214324.

[2] Yuli Yin, Fan Pan, Martina Ahlberg, Mojtaba Ranjbar, Philipp Dürrenfeld, Afshin Houshang, Mohammad Haidar, Lars Bergqvist, Ya Zhai, Randy K Dumas, Anna Delin, Johan Åkerman (2015). Tunable permalloy-based films for magnonic devices, Phys. Rev. B 92, 024427.

[3] Jonathan Chico, Corina Etz, Lars Bergqvist, Olle Eriksson, Jonas Fransson, Anna Delin, Anders Bergman (2014). Thermally driven domain-wall motion in Fe on W (110), Phys. Rev. B 90, 014434.

[4] Simone Borlenghi, Weiwei Wang, Hans Fangohr, Lars Bergqvist, Anna Delin (2014). Designing a spin-Seebeck diode, Phys. Rev. Lett. 112, 047203.

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## Exciton binding and instabilities in quasi-1d Carbon based systems

Elisa Molinari

Uni Modena e Reggio Emilia, and CNR-NANO, Modena, Italy

I will discuss the effects of dimensionality and reduced screening on electron-hole binding in selected quasi-1d Carbon based systems, as obtained from large scale Many Body Perturbation Theory calculations.

I will focus on two examples: (i) realistic graphene nanoribbons, showing strongly bound excitonic signatures in spectroscopies, and (ii) zero-gap C nanotubes where electronic correlations are predicted to induce a transition to the long-sought 'excitonic insulator' ground state, as also confirmed by quantum Monte Carlo calculations.

Work performed in collaboration with (i) Deborah Prezzi, Alice Ruini, Claudia Cardoso, and Andrea Ferretti, and (ii) Daniele Varsano, Sandro Sorella, Davide Sangalli, Matteo Barborini, Stefano Corni, and Massimo Rontani, and supported in part by Prace and by the MaX European Center of Excellence ([www.max-centre.eu](http://www.max-centre.eu)).



# Modeling Light-Matter interactions: Quantum Electrodynamics (QED) Chemistry and Materials within TDDFT

Angel Rubio

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## Abstract:

Computer simulations that predict the light-induced change in the physical and chemical properties of complex systems, molecules, nanostructures and solids usually ignore the quantum nature of light. We have recently shown how the effects of the photons can be properly included in such calculations. The basic idea is to treat the full QED system of particles and photons as a quantum fluid. Here the particles are represented by a charge current, and the photons by a classical electromagnetic field that acts on the current in a very complex manner. This study opens up the possibility to predict and control the change of material properties due to the interaction with light particles from first principles .

Here we will review the recent advances within density-functional a schemes to describe spectroscopic properties of complex systems with special emphasis to modeling time and spatially resolved electron spectroscopies We will discuss the theoretical approaches developed in the group for the characterization of matter out of equilibrium, the control material processes at the electronic level and tailor material properties, and master energy and information on the nanoscale to propose new devices with capabilities. We will focus on examples linked to the efficient conversion of light into electricity or chemical fuels ("artificial photosynthesis") and the design on new nanostructure based optoelectronic devices, among others.

Our goal is to provide a detailed, efficient, and at the same time accurate microscopic approach for the ab-initio description and control of the dynamics of decoherence and dissipation in quantum many-body systems. This theoretical framework provides a new way to control and alter chemical reactions in complex systems, direct the movement of electrons, selectively trigger physico-chemical processes, and create new state of mater

## Some references:

Atoms and Molecules in Cavities: From Weak to Strong Coupling in QED Chemistry, J. Flick, M. Ruggenthaler, H. Appel, A. Rubio, Proceedings of The National Academy of Sciences of The United States of America (2016)

Kohn-Sham Approach to Quantum Electrodynamical Density Functional Theory: Exact Time-Dependent Effective Potentials in Real Space J. Flick, M. Ruggenthaler, H. Appel, A. Rubio  
Proceedings of The National Academy of Sciences of The United States of America 112 15285-15290 (2015)

Optimized Effective Potential for Quantum Electrodynamics Time-Dependent Density Functional Theory  
C. Pellegrini, J. Flick, I. V. Tokatly, H. Appel and A. Rubio  
Physical Review Letters 115, 093001 (2015)

Quantum Electrodynamics Density-Functional Theory: Bridging Quantum Optics and Electronic-Structure Theory  
M. Ruggenthaler, J. Flick, C. Pellegrini, H. Appel, I. V. Tokatly, A. Rubio  
Physical Review A 90 012508-1,26 (2014)

Coherent ultrafast charge transfer in an organic photovoltaic blend  
S. Maria Falke, C.A. Rozzi, D. Brida, M. Amato, A. De Sio, A. Rubio, G. Cerullo, E. Molinari, C. Lienau,  
Science 344 1001-1005 (2014)



**Title: Coupled-cluster theory for condensed-phase spectroscopy**

**Timothy Berkelbach**  
the University of Chicago  
Dept. of Chemistry  
berkelbach@uchicago.edu

Abstract:

Wave function-based quantum chemistry techniques, such as MP2 and coupled-cluster theory, are starting to be applied to condensed-phase materials, leading to accurate and controlled treatments of electron correlation. I will describe the first applications of excited-state coupled-cluster theory (so-called equation-of-motion coupled-cluster) to systems with explicit periodicity. This approach represents a departure from time-dependent diagrammatic Green's function techniques like the GW approximation. In particular, I will present results for the spectral function of the paradigmatic uniform electron gas, where equation-of-motion coupled-cluster theory correctly produces satellite structure due to electron-plasmon coupling and yields a quasiparticle bandwidth in good agreement with experimental photoemission data; these results are compared with those obtained from the GW and GW+cumulant approximations. I will also present results for the quasiparticle band structure and band gaps of fully atomistic solids such as diamond and silicon. Both formal and computational aspects of the approach, including the relation to the GW approximation, will be discussed.

**Title: Excited-State Phenomena in Organic Materials and  
at Interfaces from First Principles**

**Jeffrey B. Neaton**

Department of Physics, University of California, Berkeley  
Molecular Foundry, Lawrence Berkeley National Laboratory

*Abstract:*

Organic semiconductors are highly tunable, chemically diverse cheap-to-process materials with promise for next-generation optoelectronics. They also harbor interesting excited-state phenomena such as singlet fission, whereby a singlet exciton decays into two spin-correlated triplets, a mechanism of significant interest for achieving efficiencies beyond the Shockley-Queisser limit of conventional solar cells. Further development of new organic materials requires new intuition that links atomic- and molecular-scale morphology to underlying excited-state properties and phenomena, and integrated studies involving theory and experiments. In this talk, I will discuss two classes of new ab initio methods for calculating excited-state properties of organic crystalline solids and interfaces. First, I will describe the use of a predictive, first-principles Bethe-Salpeter framework for understanding the morphology dependence of multiexciton effects, such as singlet fission, in acene crystals, such as pentacene, tetracene, and TIPS-pentacene. Second, I will cover the use of a new class of tuned hybrid functionals for predicting spectroscopic properties of acene crystals and level alignment at metal-molecule interfaces with density functional theory. Direct connections with experiments will be drawn in all cases.



**Title: A High-Throughput Computational Search for New Transparent Conducting Oxides and New Thermoelectrics**

**Gian-Marco Rignanese**

Universite Catholique de Louvain  
Institut de la matière Condensée et des Nanosciences  
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B-1348 Louvain La Neuve, Belgium

Abstract:

Many essential materials properties can nowadays be computed using ab initio methods. When coupled with the exponential rise in computational power available to research groups, this predictive power provides the opportunity for large-scale computational searches for new materials. Tens of thousands of novel materials can be generated and screened by their computed properties even before their synthesis, focusing experiments on the most promising candidates and exploring rapidly new chemical spaces. We will present the potential of such high-throughput calculations for searching for new high-performance transparent conducting oxides (TCOs) and thermoelectrics.

TCOs are critical to many technologies from solar cells to electronics. However, finding materials that combine the two antagonistic properties of large conductivity and transparency to the visible light can be extremely challenging. Combining different ab initio techniques from density functional theory to many-body perturbation theory, we evaluated thousands of oxides in terms of essential TCO properties (e.g., band gap and carrier transport). From these results, we will present interesting new compounds as well as discuss the chemistries likely to form high performance TCOs. We will focus on  $Ba_2BiTaO_6$  which we proposed as a potential high-mobility, visibly transparent p-type oxide using our high-throughput computational screening and which was synthesized and characterized as such experimentally. Finally, we will discuss the influence of the "second gap" on the transparency of TCOs.

Thermoelectrics are promising for addressing energy issues but their exploitation is still hampered by low efficiencies. So far, much improvement has been achieved by reducing the thermal conductivity but less by maximizing the power factor. The latter imposes apparently conflicting requirements on the band structure: a narrow energy distribution and a low effective mass. We will describe an original approach to fulfill both requirements in bulk semiconductors. It exploits the highly directional character of some orbitals to engineer the band structure and produce a type of low-dimensional transport similar to that targeted in nanostructures, while retaining isotropic properties [6]. We will then present an overview and preliminary analysis of thermoelectric properties computed with the BoltzTraP code for more than 48000 inorganic compounds from the Materials Project. Finally, we will focus on a new group of thermoelectric materials which have been discovered by the high-throughput screening and which were also investigated experimentally.



# Atomistic Structure Prediction via Swarm Intelligence Algorithms

Yanming Ma

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Knowledge of atomistic structures is essential if the properties of materials are to be understood and exploited, particularly when establishing a correspondence between materials performance and their chemical compositions. Precise prediction of atomistic structures with the given information of chemical compositions is highly desirable, but it is extremely difficult as it basically involves in exploring a huge number of energy minima on the high-dimensional potential energy surface. There is an urge on development of global optimization algorithms on efficient exploration of energy surface to identify the global stable structure.

We have developed an efficient CALYPSO structure prediction approach [1-2] via multi-objective swarm-intelligence optimization algorithms by taking the advantage of structures smart learning where both particle swarm optimization and artificial bee colony algorithms are employed (See more information at <http://www.calypso.cn>). The method has been widely used by more than 1600 users to design multi-dimensional structures ranging from 3D bulk crystals to 0D nanoclusters, 2D layers and surfaces, etc [3-5]. Functionality-driven inverse design of electride, superhard, and optical materials are also feasible [6].

CALYPSO has played a leading role in major high-pressure experimental discoveries. Predicted chemical reactions of Fe/Ni and Xe at the conditions of Earth core [7] and its experimental confirmation might provide a possible solution on “missing Xe paradox” towards to the Xe storage in the Earth Core. Our prediction of high-Tc superconductivity of H<sub>2</sub>S [8] has initiated the exciting experimental discovery of record high 200 K superconductivity on highly compressed H<sub>2</sub>S.

## References:

- [1] Y. Wang, J. Lv, L. Zhu, and Y. Ma, Phys. Rev. B 82, 094116 (2010).
- [2] Y. Wang, J. Lv, L. Zhu, and Y. Ma, Comput. Phys. Commun. 183, 2063 (2012).
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- [5] Y. Wang, et al., J. Chem. Phys. 137, 224108 (2012).
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- [7] L. Zhu, H. Liu, C. Pickard, G. Zou, and Y. Ma, Nature Chem. 6, 644 (2014).

**Title: Topological Electronic States and Materials**

**Author: Zhong Fang**

**Affiliation: Institute of Physics, Chinese Academy of Sciences, Beijing  
100190, China**

Abstract:

The rapid development in the field of topological states is due both to conceptual theoretical advances, and to the discoveries of realistic materials where these exotic states can be hosted. First principles calculations play important roles in this field. On the theoretical front, the calculations and understanding of Berry curvature and gauge field established the connection between topology and electronic structures. On the experimental side, most of materials discovered up to now in this field are stimulated by computational predictions. In this talk, I will review recent progresses in this field, with focus on topological semimetals, and address some recent theoretical and experimental results.



# Emergent Behavior in Thermal Transport

Andrea Cepellotti

*Theory and simulation of materials (THEOS) and National Center for Computational Design and Discovery of Novel Materials (MARVEL), École Polytechnique Fédérale de Lausanne, Switzerland*

*University of California, Berkeley, and Lawrence Berkeley National Laboratory, USA*

The thermal conductivity of insulating crystals originates from the energy transfer through lattice vibrations, as commonly described by the phonon Boltzmann transport equation. Since the pioneering work of Peierls, the prevalent hypothesis is that phonons are the heat carriers. However, it has long been known that this picture has shortcomings. For example, in materials of reduced dimensionality [1] or at cryogenic temperatures, the scattering dynamics is dominated by momentum conserving – normal – processes, as opposed to momentum dissipating – Umklapp – processes. In these circumstances, heat flux is not lost at every scattering event. Instead, scattering shuttles heat flux through multiple phonon states, coupling them. As a result, the behavior of the interacting phonon system can be strikingly different from that of its constituents and collective phonon excitations arise [2] causing exotic phenomena: in 2D materials, they are responsible of high thermal conductivities and hydrodynamic behaviors, such as second sound [1,3], where temperature propagates as a damped wave, a phenomenon hitherto observed only in a few materials at cryogenic temperatures. Recently, we rationalized these properties by introducing a gas of collective phonon excitations, called ‘relaxons’ [4]. Defined as the eigenvectors of the scattering matrix, relaxons allow for a simple - yet exact - interpretation of thermal conductivity in terms of a kinetic gas theory, where the relevant gas is made of such relaxons, the true heat carriers, and not phonons. These considerations provide a new explanation of the high conductivities of 2D materials, revise the time evolution of thermalization processes [5], correct the relevant time and length scale of heat flux dissipation, and provide a new viewpoint on semiclassical transport theories.

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[3] S. Lee et al., Nat. Commun., 6, 6290 (2015)

[4] A. Cepellotti, and N. Marzari Phys. Rev. X 6, 041013 (2016)

[5] J. Hu, et al., PNAS 113, 43, E6555 (2016)



**Title: Atomistic mechanisms and kinetics during phase transformations in metals**

**Jutta Rogal**

Interdisciplinary Centre for Advanced Materials Simulation, ICAMS  
Ruhr-Universität Bochum, Germany  
email: jutta.rogal@rub.de

Abstract:

Atomistic modelling of the dynamics of phase transformations is a particularly challenging task. If the mechanism of the phase transformation is governed by so-called rare events then the time scale of interest will reach far beyond the capabilities of regular molecular dynamics simulations.

One example are the atomistic rearrangements during solid-solid phase transformations in bulk systems which involve massive structural changes including concerted multi-atom processes. The interface between two structurally different phases leads to a complex energy landscape that needs to be explored during the dynamical evolution of the interface. Here, we employ an adaptive kinetic Monte Carlo (AKMC) approach to investigate such processes at the interface between the body-centered cubic and A15 phase in molybdenum.

A second example is the initial nucleation and growth during solidification in metals. Here, we investigate the atomistic mechanisms of nucleation in nickel for various undercoolings using transition path sampling (TPS). The analysis of the path ensemble reveals a non-classical behaviour with mainly non-spherical nuclei, and shows that the nucleation initiates in regions with high orientational order that also predetermine the polymorph selection.

## Improving the scalings of Quantum Monte Carlo methods, with multi-determinant expansions.

Roland Assaraf, Claudia Filippi and Saverio Moroni.

*Department of Chemistry, Université P. et M. Curie  
Paris, France*

We present recent developments of quantum Monte Carlo methods in real space, to compute efficiently many energy derivatives and observables, with a multi-determinant Jastrow-Slater wave function. The computational scaling as a function of the number  $N_e + 1$  of determinants is reduced to  $O(N_e)$  for an entire set of derivatives down from  $O(N_e)^1$  or  $O(NN_e)^2$  per derivative, where  $N$  is the number of electrons. As a function of  $N$ , the computational cost,  $O(N^{0-2})$  per derivative, extends what is obtained with the less transparent algorithmic differentiation technique for one single determinant.

- [1] C. Filippi, R. Assaraf and S. Moroni, JCP **144**, 194105 (2016).
- [2] K. Clark, M. A. Morales, J. McMinis, J. Kim, and G. E. Scuseria, J. Chem. Phys. **135**, 244105 (2011).

## Entropy as a collective variable

**Prof. Michele Parrinello**

Department of Chemistry and Applied Biosciences, ETH Zurich, and Facoltà di Informatica,  
Istituto di Scienze Computazionali, Università della Svizzera italiana, 6900 Lugano, Switzerland

### Abstract:

Sampling complex free energy surfaces that exhibit long lived metastable states separated by kinetic bottlenecks is one of the most pressing issues in the atomistic simulations of matter. Not surprisingly many solutions to this problem have been suggested. Many of them are based on the identification of appropriate collective variables that span the manifold of the slow varying modes of the system. While much effort has been put in devising and even constructing on the fly appropriate collective variables there is still a cogent need of introducing simple, generic, physically transparent, and yet effective collective variables. Motivated by the physical observation that in many case transitions between one metastable state and another result from a trade off between enthalpy and entropy we introduce appropriate collective variables that are able to represent in a simple way these two physical properties. We use these variables in the context of the recently introduced variationally enhanced sampling and apply it them with success to the simulation of crystallization from the liquid and to conformational transitions in protein.



**Title: "Car and Parrinello meet Green and Kubo: simulating atomic heat transport from equilibrium ab initio molecular dynamics"**

**Stefano Baroni**  
SISSA, Trieste

Abstract:

Modern simulation methods based on electronic-structure theory have long been deemed unfit to compute heat transport coefficients within the Green-Kubo formalism. This is so because the quantum-mechanical energy density from which the heat flux is derived is inherently ill defined, thus allegedly hampering the use of the Green-Kubo formula. While this objection would actually apply to classical systems as well, I will demonstrate that the thermal conductivity is indeed independent of the specific microscopic expression for the energy density and current from which it is derived. This independence results from a kind of *gauge invariance* stemming from energy conservation and extensivity, which I will illustrate numerically for a classical Lennard-Jones fluid. I will then introduce an expression for the adiabatic energy flux, derived within density-functional theory, that permits the ab initio simulation of atomic thermal transport using equilibrium molecular dynamics. The resulting methodology is demonstrated by comparing results from ab-initio and classical molecular-dynamics simulations of a model liquid-Argon system, for which accurate inter-atomic potentials are derived by the force-matching method, and applied to compute the thermal conductivity of heavy water at ambient conditions. The problem of evaluating transport coefficients along with their accuracy from relatively short trajectories is finally addressed and discussed with a few representative examples.

## Non-locality in lattice thermal conductivity

Philip B. Allen

Stony Brook University, New York, USA

Phonons  $Q = (\vec{Q}, j)$  in crystals have very slow relaxation rates  $1/\tau_Q$  at long-wavelength (small  $Q$ ). This causes the heat current  $j(x)$  to depend on the temperature gradient  $dT(x')/dx'$  at long distances  $|x - x'|$ . In a homogeneous crystal, the non-local conductivity  $\kappa(x, x')$  depends only on  $x - x'$ ; the Fourier-space representation  $j(q) = -\kappa(q)dT/dx(q)$  is helpful for analysis. I use this to analyze simulations (Zhou *et al.*, Phys. Rev. B **79**, 115201 (2009), Liang *et al.*, J. Appl. Phys. **118**, 125104 (2015)) of GaN thermal conductivity. The Peierls-Boltzmann equation in relaxation time approximation gives a formula for  $\kappa(q)$ . Using a Debye model, explicit results  $\kappa_p(q)$  are found for models where  $1/\tau_Q \propto Q^p$ . Numerics often gives exponents  $p$  to be 2, 3, or 4. When  $p = 2$ ,  $\kappa_2(q) \sim \kappa_0 - C\sqrt{q}$ . This shows that simulations on samples of size  $L$  should be extrapolated by plotting  $\kappa(L)$  versus  $1/\sqrt{L}$ . For exponent  $p \geq 3$ ,  $\kappa(q)$  diverges as  $q \rightarrow 0$ , which means that  $\kappa(L)$  diverges as  $L \rightarrow \infty$ . An improved analysis is described, which uses Callaway's version of the relaxation time approximation, treating  $N$  and  $U$  processes separately.

# One-shot calculation of temperature-dependent optical spectra and phonon-induced band-gap renormalization

*Feliciano Giustino*

Department of Materials, University of Oxford

The calculation of the electronic and optical properties of solids is usually performed by describing the nuclei as classical particles clamped to their equilibrium positions. This approximation inevitably misses the dependence of electronic and optical properties on temperature, quantum zero-point effects, and phonon-assisted optical processes [1]. In this talk I will introduce a recent development, the Williams-Lax theory, which enables the calculation of the temperature-dependent optical spectra and band gaps of solids by seamlessly including quantum nuclear effects and phonon-assisted transitions [2]. The optical absorption coefficients of common semiconductors calculated using this technique are in remarkable agreement with experiments over several orders of magnitude, both for direct-gap semiconductors like gallium arsenide and for indirect-gap semiconductors like silicon. I will show how the Williams-Lax theory is related to the theory of temperature-dependent band structures by Allen and Heine, and provides an adiabatic approximation to the classic theory of phonon-assisted optical absorption by Hall, Bardeen, and Blatt. I will also discuss how this theory relates to imaginary-time path integrals. The main advantage of this new approach is that it enables the calculation of optical properties of solids at finite temperature using a single supercell calculation (one-shot) [3]. Since the Williams-Lax method is agnostic to the theory employed for describing electronic and optical excitations, it can also be used for performing systematic GW/BSE calculations at finite temperature.

[1] F. Giustino, *Rev. Mod. Phys.* 2017, in press; [arXiv:1603.06965](https://arxiv.org/abs/1603.06965).

[2] M. Zacharias, C. E. Patrick, and F. Giustino, *Phys. Rev. Lett.* 115, 177401 (2015).

[3] M. Zacharias and F. Giustino, *Phys. Rev. B* 94, 075125 (2016).



**Title: Advances in semi-empirical density functionals for molecules and materials**

**Martin Head-Gordon**

Kenneth S. Pitzer Distinguished Professor, Dept. of Chemistry, Univ. of California,  
Berkeley, and,  
Senior Faculty Scientist, Chemical Sciences Division, Lawrence Berkeley  
National Laboratory  
USA

**Abstract:**

I shall discuss progress in the design of a next generation of density functional theories. In contrast to most approaches to functional design, we have adopted a combinatorial approach, in which we have trained a huge number of functionals (over 100,000 in the case of the generalized gradient approximation models, and over  $10^{10}$  in the case of meta GGA functionals). The functional from each class that performs best on independent test data (survival of the most transferable) is self-consistently trained to yield new generation functionals that seems very promising for application purposes. A key component of these functionals is the non-local VV10 density-density correlation functional that enables highly accurate treatment of non-bonded interactions, if the entire functional is self-consistently trained. The resulting functionals involve significantly fewer parameters than many of the best functionals of recent years. I shall discuss the results of large-scale benchmarking exercises that assess the new functionals against other existing functionals.

**TITLE: Electron correlation from the adiabatic-connection-fluctuation-dissipation-theorem approach for a multireference wavefunction.**

**Katarzyna Pernal**  
Institute of Physics  
Lodz University of Technology  
Lodz, Poland

**ABSTRACT:**

In the first part of the talk I will present a general formalism that employs adiabatic connection formula and the fluctuation dissipation theorem that leads to a correlation functional if single-reference and some multireference wavefunctions are used. Then the formalism will be employed in connection with the strongly orthogonal geminal model to describe subtle correlation effects in weakly interacting multireference systems. Such systems require proper description of the long-range dynamic correlation together with the long-range static effects. They pose a serious challenge for a coupled cluster CCSD(T) method and a multireference CASPT2 approach.

Strongly Constrained and Appropriately Normed (SCAN) Semilocal Density Functional:  
Accurate and Efficient for Structures and Energies of Diversely-Bonded Materials

Jianwei Sun

Department of Physics

The University of Texas at El Paso

In condensed matter physics, materials science, and chemistry, it is of critical importance to know if one atom or molecule can bind to another and with how much energy. The strengths of different types of bonds between atoms and molecules can vary from several meV to several eV. Although some first-principles methods can provide accurate descriptions of all bond types, those methods are not efficient enough for studies of complex systems (e.g., large systems, *ab initio* molecular dynamics, and high-throughput searches for functional materials). We show here that the recently developed non-empirical strongly constrained and appropriately normed (SCAN) [1] meta-generalized gradient approximation (meta-GGA) within the density functional theory framework predicts accurate geometries and energies of diversely-bonded molecules and materials (including covalent, metallic, ionic, hydrogen, and van der Waals bonds), significantly improving over its predecessors, at comparable efficiency, the GGAs that dominate materials computation [2]. SCAN is the first meta-GGA that is fully constrained, obeying all 17 known exact constraints that a meta-GGA can. The meta-GGA is also exact or nearly exact for a set of “appropriate norms”, where the exact exchange- correlation hole is localized near its electron. Remarkably, SCAN often matches or improves upon the accuracy of a computationally expensive hybrid functional, at almost-GGA cost. Two error sources, i.e., the long-range vdW interaction and the self-interaction error, intrinsic to any semilocal density functionals to which SCAN belongs, however remain. The addition of the long-range vdW correction to SCAN [3] results in a versatile vdW functional that is accurate and outperforms its competitors for a variety of vdW-dominated systems, including layered materials and organic molecules adsorbed on metal surfaces.

[1] J. Sun, A. Ruzsinszky, and J.P. Perdew, Strongly constrained and appropriately normed semilocal density functional, *PRL* **115**, 036402 (2015).

[2] J. Sun, R.C. Remsing, Y. Zhang, Z. Sun, A. Ruzsinszky, H. Peng, Z. Yang, A. Paul, U. Waghmare, X. Wu, M.L. Klein, and J.P. Perdew, Accurate First-principles structures and energies of diversely-bonded systems from an efficient density functional, *Nat. Chem.* **8**, 831 (2016).

[3] H. Peng, Z. Yang, J.P. Perdew, and J. Sun, Versatile van der Waals density functional based on a meta-generalized gradient approximation, *PRX* **6**, 041005 (2016).



**Title: Large Scale Many-Body Perturbation Theory Calculations:  
Methodological Developments, Data Collections, Validation and  
Applications**

**Marco Govoni, PhD.**

Assistant Scientist

Materials Science Division

Argonne National Laboratory

Argonne, IL 60439

[mgovoni@anl.gov](mailto:mgovoni@anl.gov)

&

Visiting Scientist

Institute for Molecular Engineering

The University of Chicago

William Eckhardt Research Center (ERC), 351

Chicago, IL 60637

[mgovoni@uchicago.edu](mailto:mgovoni@uchicago.edu)

**Abstract:**

One of the main tools used in first principle simulations of materials is Density Functional Theory; however, several of the approximate exchange and correlation functionals do not provide the level of accuracy required for predictive calculations of excited state properties. The application to large systems of more accurate post-DFT approaches such as Many-Body Perturbation Theory (MBPT) – for example to heterogeneous systems, nanostructured, disordered, and defective materials – has been hindered by high computational costs. In this talk recent methodological developments in MBPT calculations will be discussed, as implemented in the open source code WEST [1]. Results using a formulation that does not require the explicit calculation of virtual states will be presented, e.g. for aqueous solutions and spin defects in insulators [2]. We will discuss online data collections which contain benchmarking results. Simplifications of MBPT calculations based on the use of static response properties, such as dielectric-dependent hybrid functionals [3], will also be presented. We will also briefly discuss the ongoing activities of the Midwest Integrated Center for Computational Materials (MICCoM).

[1] [www.west-code.org](http://www.west-code.org); M. Govoni et al., J. Chem. Theory Comput. 11, 2680 (2015).

[2] A. Gaiduk et al., J. Am. Chem. Soc. Commun. 138, 6912 (2016); H. Seo et al., Sci. Rep. 6, 20803 (2016); P. Scherpelz et al., J. Chem. Theory Comput. 12, 3523 (2016).

[3] J.H. Skone et al., Phys. Rev. B 89, 195112 (2014); J.H. Skone et al., Phys. Rev. B 93, 235106 (2016); N. Brawand et al., Phys. Rev. X 6, 041002 (2016).

**TITLES OF  
POSTERS**

## **POSTER SESSION I**

**THURSDAY, JANUARY 12, 2017**

**The full abstract can be found on the Workshop's website:**

**<http://indico.ictp.it/event/7948/>**



## POSTER SESSION I

**THURSDAY, JANUARY 12, 2017**  
**18:00, Adriatico Guesthouse, Lower Level**

### **A - L In alphabetical order by Author**

**1) Title: Water on graphene oxide: steps toward understanding ultrafast proton transport theoretically**

**Debdipto Acharya**, Jawaharlal Nehru Centre For Advanced Scientific Research  
Bangalore, India

**2) Title: Stability of Pt-Ru alloy for anode catalyst and CO tolerance mechanism in PEFC Fuel Cell using combined DFT and Monte Carlo Simulation**

**Md Khorshed Alam**, Daffodil International University, Department of Natural Sciences  
Faculty of Science and Information Technology, Dattapara, Savar, Dhaka

**3) Title: Vacancy in graphene nano-flakes: a first principles study**

**A.M.Valencia<sup>1</sup> and M.J.Caldas<sup>1</sup>**, <sup>1</sup>Institute of Physics, University of São Paulo, São Paulo, Brazil

**4) Title: Physical adsorption: Nanoscale van der Waals interactions beyond the Lifshitz-Zaremba-Kohn limit**

**Alberto Ambrosetti**, Università di Padova, Padova, Italy

**5) Title: Giant magnetoelectricity in Ni<sub>3</sub>TeO<sub>6</sub> from first principles**

**Sergey Artyukhin**, Italian Institute of Technology, Quantum Materials Theory group  
Genova, Italy

**6) Title: Anharmonicity and the isotope effect in superconducting lithium at high pressures: a first-principles approach**

**Unai Aseginolaza Aguirreche**, Material Physics Center (MPC), San Sebastian, Spain

**7) Title: Electronic and Optical properties of hydrogenated TiO<sub>2</sub>**

**Samaneh Ataei Seyedeh**, University of Tehran, Department of Physics, Tehran, Iran

**8) Title: First Principle Calculations of LiRh<sub>2</sub>Ge and LiCu<sub>2</sub>Ge Heusler Alloys**

**Seyfettin Ayhan**, Graduate School of Natural and Applied Science, Diyarbakir, Turkey

**9) Title: Ab-initio Raman spectroscopy within the DFPT+PAW formalism**

**Lucas Baguet**, CEA, DAM, DIF, Arpajon, France

**10) Title: One-shot calculation of complete low pressure phase diagrams.**

**Robert Baldock**, EPFL, School of Engineering, Institute of Materials, Theory and Simulation of Materials, Lausanne, Switzerland

**11) Title: High-throughput screening of binary oxides to discover intermediate band compounds**

**Douglas Baquião Ribeiro**, UFABC, Santo André, Brazil

12) Title: **Ab initio study of structural, electronic and hydriding properties of FeTi intermetallic**

**Fatima-Zohra Bentayeb**, Physics Department, Annaba, Algeria

13) Title: **A first-principles study of liquid and amorphous phases of the In<sub>2</sub>Te<sub>3</sub> compound**

**Marco Bernasconi**, Universita' degli Studi di Milano Bicocca, Dip. Scienza dei Materiali  
Milano, Italy

14) Title: **B1-B2 phase transition of LiH at finite temperature**

**Sananda Biswas**, Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR)  
Bangalore, Karnataka, India

15) Title: **Quasiparticle band structure and optical properties of hexagonal-YMnO<sub>3</sub>**

**Tathagata Biswas**, Center for Condensed Matter Theory, Department of Physics  
Indian Institute of Science, Bangalore, Karnataka, India

16) Title: **Anharmonic enhancement of superconductivity in molecular hydrogen at high pressure**

**Miguel Borinaga**, Centro de Fisica de Materiales, CFM-MPC CSIC-EHU, Donostia San Sebastian  
Spain

17) Title: **Mechanistic study of zeolite -catalysed dehydration of ethanol to ethylene (formation of the likely precursor for hydrocarbons.)**

**Cecil Botchway**, Kwame Nkrumah University of Science and Technology, Kumasi, Ghana

18) Title: **Doping, co-doping, and defect effects on the plasmonic activity of ZnO-based transparent conductive oxides**

**Arrigo Calzolari**, Istituto Nanoscienze CNR NANO S3, Modena, Italy

19) Title: **Computational design of novel 2d-materials for electronic applications**

**Davide Campi**, Ecole polytechnique fédérale de Lausanne (EPFL) STI THEOS, Lausanne, Switzerland

20) Title: **ATOMIC SCALE INVESTIGATION OF GRAPHENE MOIRE' STRUCTURES ON NI(100)**

**Virginia Carnevali**, Universita degli Studi di Trieste, Department of Physics, Trieste, Italy

21) Title: **Ab-initio molecular dynamics simulations of polaron- and exciton- induced OLED degradation**

**Marco Cazzaniga**, Istituto di Scienze e Tecnologie Molecolari, Consiglio Nazionale delle Ricerche, CNR,  
Milano, Italy

22) Title: **Organic functionalization of MoS<sub>2</sub> monolayer**

**Giancarlo Cicero**, Politecnico of Torino, Torino, Italy

23) Title: **Koopmans-compliant functionals: A reliable and efficient tool for spectroscopic quantities.**

**Nicola Colonna**, Ecole Polytechnique federale de Lausanne (EPFL), Lausanne, Switzerland

24) Title: **Thermal energy storage in nanofluids: what can simulations teach us?**

**Francesca Costanzo**, Cataln Institute of Nanoscience and Nanotechnology, Barcelona, Spain



- 25) Title: **Graphene-based synthetic antiferromagnets: an ab-initio study**  
**Ramón Cuadrado del Burgo**, Theory and Simulation Group, Institut Català de Nanociència i Nanotecnologia (ICN2), Barcelona, Spain
- 26) Title: **Symmetry classification of the electronic states and of the normal vibrational modes of a solid using the projective representations of the point group: a numerical implementation**  
**Andrea Dal Corso**, International School for Advanced Studies SISSA-ISAS, Condensed Matter Sector, Trieste, Italy
- 27) Title: **X atoms inserted in hematite photoanodes for enhancing photoelectrochemical activity: An ab initio prediction**  
**Bruno Dandogbessi**, African University of Science and Technology, Abuja, Nigeria
- 28) Title: **Machine-learning based interatomic potential for amorphous carbon**  
**Volker Deringer**, University of Cambridge, Department of Engineering and Department of Chemistry, Cambridge, United Kingdom
- 29) Title: **Strong correlation in Double-Perovskites using DFT+U**  
**Mostefa Djermouni**, University Djilali Liabès of Sidi Bel-Abbès, Sidi Bel-Abbès, Algeria
- 30) Title: **Gaussian approximation potentials for  $\alpha$ -iron**  
**Daniele Dragoni**, Università degli Studi di Milano - Bicocca, Dipartimento di Scienze dei materiali, Milano, Italy
- 31) Title: **A downfolded effective Hamiltonian combining MBPT with quantum chemistry**  
**Marc Dvora**, Aalto University, Espoo, Finland
- 32) Title: **Competing Structures in (In,Ga)Se and (In,Ga)<sub>2</sub>Se<sub>3</sub> Semiconductors**  
**Fouad El Haj Hassan**, Lebanese University, Faculty of sciences, Department of Physics  
Laboratoire de Physique et d'Electronique (LPE), Beirut, Lebanon
- 33) Title: **the Impact of the presence of off-center confined alkali atom on C60**  
**Anne Justine Etindele**, University of Douala, Faculty of Sciences, Department of physics  
Laboratory of Fundamental Physics, Douala, Rep. of Cameroon
- 34) Title: **Ab initio quality neural network potential for CaF<sub>2</sub> based on charge equilibration process**  
**Somayeh Faraji Nafchi**, Institute for Advanced Studies in Basic Sciences (IASBS)  
Zanjan, Iran
- 35) Title: **Toward the non-equilibrium Green's function calculation based on a divide-conquer approach**  
**Mashiro Fukuda**, Institute for Solid State Physics, University of Tokyo, Ozaki Laboratory, Chiba, Japan
- 36) Title: **Structural Relaxations and Resistance Drift in Amorphous GeTe from Atomistic Simulations**  
**Silvia Gabardi**, Università degli Studi di Milano-Bicocca, Dipartimento di Scienza dei Materiali Milano, Italy



37) Title: **One-dimensional metallic wires at phase-engineered boundaries in two-dimensional materials**

**Marco Gibertini**, École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland

38) Title: **Local density fitting within a Gaussian and plane waves approach to enable large-scale DFT simulations**

**Dorothea Golze**, Aalto University, Department of Applied Physics, COMP Centre, Espoo, Helsinki, Finland

39) Title: **Electronic and optical properties of Weyl semimetals based on transition metal monpnictides: Ab initio studies of TaAs, TaP, NbAs and NbP**

**Davide Grassano**, Universita' degli studi di Roma Tor Vergata, Rome, Italy

40) Title: **Charge-Density-Wave state in TiSe<sub>2</sub> single-layers**

**Ionel Guster**, Catalan Institute of Nanoscience and Nanotechnology, Bellaterra, Cerdanyola del Valles Barcelona, Spain

41) Title: **Metallic nanoparticles under realistic electrochemical conditions**

**Nicolas Hoermann**, Theory and Simulation of Materials (THEOS), EPFL, Lausanne, Switzerland

42) Title: **Computational Methods in Elucidating Mechanisms of Heterogeneous Catalysis**

**Matej Huš**, National Institute of Chemistry, Department of Catalysis and Chemical Reaction Engineering, Ljubljana, Slovenia

43) Title: **Hybrid functional study of P, As, Sb and Bi induced defect levels in Ge**

**Emmanuel Igumbor**, Samuel Adegboyega University, Ogwa-Edo, Nigeria

44) Title: **Thermal conductivity of 2D materials from first principles**

**Sergio Illera**, Consejo superior de investigaciones científicas (CSIC) ICMA, Bellaterra, Spain

45) Title: **First-principles study of anomalous Nernst effect in skyrmion crystals**

**Fumiyuki Ishii**, Kanazawa University, Kanazawa, Japan

46) Title: **First principles study of electron scattering mechanism at SiC/SiO<sub>2</sub> interface**

**Shigeru Iwase**, Department of Pure and Applied Sciences, University of Tsukuba, Tsukuba, Obaraki, Japan

47) Title: **2D Structures of III-VI Materials in Non-Hexagonal Symmetry**

**Olmos Asar Jimena**, Centro de Ciências Naturais e Humanas - UFABC, Santo André, Brazil

48) Title: **Lattice matched interfaces between semiconductor alloys and metals**

**Line Jelver**, Technical University of Denmark, Lyngby, Denmark

49) Title: **Self-Interaction Effects of Transition Metal Phthalocyanines on Graphene: A DFT Study**

**Apichai Jomphoak**, Maezono Group, Electronic Structure Calculation Group at JAIST, Ishikawa, Japan

50) Title: **Two-dimensional electron gases at head-to-head and tail-to-tail domain walls in ferroelectric thin films**

**Francisco Javier Junquera Quintana**, Universidad de Cantabria, Departamento de Ciencias de la Tierra y Física de la Materia Condensada, Santander, Spain

51) Title: **The pinball model - A framework for the search for solid-state electrolytes**  
**Leonid Kahle**, Theory and Simulation Laboratory (THEOS), Ecole Polytechnique Federal de Lausanne (EPFL), Lausanne, Switzerland

52) Title: **Quantum mechanical simulation of cobalt based magnetic coverages on two dimensional WS<sub>2</sub> semiconductor**  
**Hamideh Kahnouji**, Isfahan University Of Technology, Department of Physics, Isfahan, Iran

53) Title: **DFT study of fundamental properties of  $\alpha'$ -Fe<sub>16</sub>C<sub>2</sub> phase and martensite decomposition at low temperature**  
**Dmytro Kandaskalov**, IM2NP, Marseille, France

54) Title: **vdW-DF + U description of solid oxygen at low pressure**  
**Shusuke Kasamatsu**, The Institute for Solid State Physics, the University of Tokyo Chiba, Japan

55) Title: **Atomic-scale investigation of grain boundary motion in graphene**  
**Dongwook Kim**, Seoul National University, Seoul, Rep. of Korea

56) Title: **Electronic and ionic transport of ions in water confined in carbon nanotubes: a combined first principles calculations**  
**Alexsandro Kirch**, Universidade de São Paulo, São Paulo, Brazil

57) Title: **Ab Initio Statistical Mechanics of Martensitic Phase Transition in NiTi Shape Memory Alloy (SMA)**  
**Pawan Kumar**, Materials Theory Group, Theoretical Sciences Unit, Jawaharlal Nehru Center For Advanced Scientific Research, Bangalore, India

58) Title: **First-principles studies of valence band structure, core level binding energy, and phonon dispersion of epitaxial silicene on zirconium diboride (0001) surface**  
**Chi-Cheng Lee**, Institute for Solid State Physics, The University of Tokyo, Kashiwa city, Japan

59) Title: **Enhanced magnetoelectric coupling in multiferroics from atomistic simulations**  
**Sergey Lisenkov**, Department of Physics, University of South Florida, Tampa, USA

60) Title: **Modeling Thiolate-Gold interface for protected nanoparticles**  
**Martin Luduena**, Universidad de Cordoba - Faculty of Chemistry, Cordoba, Argentina

61) Title: **Indiene - a new monolayer material**  
**Igor Lukačević**, University of Zagreb, Zagreb, Croatia



## **POSTER SESSION II**

**FRIDAY, JANUARY 13, 2017**

**The full abstract can be found on the Workshop's website:**

**<http://indico.ictp.it/event/7948/>**



## POSTER SESSION II

FRIDAY, JANUARY 13, 2017

18:00, Adriatico Guesthouse, Lower Level

### M - Z in alphabetical order by Author

1) Title: **Electronic properties of BN-doped T graphene: A density functional theory study**

**Roya Majidi**, Department of Physics, Shahid Rajaei Teacher Training University, Tehran, Iran

2) Title: **Electronic and optical properties of hexathiapentacene in the gas and crystal phases**

**Giuliano Mallocci**, Dipartimento di Fisica, Università degli Studi di Cagliari, Monserrato, Italy

3) Title: **High-throughput search for Z2 topological insulators in two dimensions**

**Antimo Marrazzo \***, co-Authors: **Marco Gibertini, Nicolas Mounet, Davide Campi and Nicola Marzari** \* Theory and Simulation of Materials (THEOS), École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland

4) Title: **Electronic and magnetic properties of zigzag graphene nanoribbons deposited on the topological insulator Sb<sub>2</sub>Te<sub>3</sub>**

**Riccardo Mazzarello**, RWTH Aachen, Institute for Theoretical Solid State Physics, Aachen, Germany

5) Title: **Accelerating ab-initio Molecular Dynamics and probing the weak dispersive forces in dense liquid hydrogen**

**Guglielmo Mazzola**, ETH Zurich, Switzerland

6) Title: **A first principles view of nanoaggregation of asphaltenes and their adsorption processes on carbonate surfaces**

**Caetano Miranda**, University of Sao Paulo, Institute of Physics, Department of Mechanics and Materials Physics, São Paulo, Brazil

7) Title: **Dimensionality effects on magnetic properties of Fe<sub>x</sub>Co<sub>1-x</sub> nanoclusters on Pt(111): an ab initio investigation**

**Ivan Miranda**, University of São Paulo, Department of Mechanics and Materials Physics (DFMT), São Paulo, Brazil

8) Title: **Mechanistic Insight into the Chemical Exfoliation and Functionalization of Ti<sub>3</sub>C<sub>2</sub>MXene**

**Avanish Mishra**, Materials Research Centre, Indian Institute of Science, Bangalore, India

9) Title: **First Principle study of CO<sub>2</sub> adsorption on TiO<sub>2</sub> surface with and without a Graphene Overlayer**

**Shashi Mishra**, (Dr. Ranjit Kumar Nanda, Associate Professor), Condensed Matter Theory and Computational Laboratory, Department of Physics, IIT - Madras, Chennai, India

10) Title: **Large-scale first-principles study of Si/Ge core-shell nanowires using a linear-scaling technique.**

**Tsuyoshi Miyazaki**, International Center for Materials Nanoarchitectonics (MANA), National Institute for Materials Science, Tsukuba, Japan

11) Title: **The electronic structure of water from Koopmans-compliant functionals**

**James Moraes de Almeida**, THEOS Theory and Simulations of Materials, Ecole Polytechnique Federale de Lausanne, Lausanne, Switzerland

12) Title: **Computational exfoliation of all known 3D materials**

**Nicolas Mounet**, Ecole Polytechnique Federale de Lausanne, Institute of Materials, School of Engineering, Theory and Simulation of Materials, Lausanne, Switzerland

13) Title: **Defect Induced magnetization in Graphene**

**Ebrahim Nadimi**, K. N. Toosi University of Technology, Tehran, Iran

14) Title: **Including the effects of atomic bonding in TEM and STEM image simulations**

**Timothy Naginey**, Materials Modelling Laboratory, Department of Materials, University of Oxford, Oxford, United Kingdom

15) Title: **How does hydrogen peroxide dissociate on Pd-M (M= Cu, Pt) alloy clusters?**

**Masoud Nahali**, Babol University of Technology, Babol, Iran

16) Title: **Optimized multi-site local orbitals in the large-scale DFT code CONQUEST**

**Ayako Nakata**, First-principles Simulation Group, Nano-Theory Field, International Center for Materials Nanoarchitectonics (MANA), National Institute for Materials Science, Tsukuba, Japan

17) Title: **Electronic and optical properties of 2D/3D heterojunctions**

**Mahesh Neupane**, US Army Research Laboratory, Aberdeen Proving Ground, USA

18) Title: **Excitons and optical spectra of phosphorene nanoribbons**

**Zahra Nourbakhsh**, Institute for Research in Fundamental Science IPM, Tehran, Iran

19) Title: **Density functional based study of boronitrene and its derivatives**

**KO Obodo (1, JT Obodo (2, RC Andrew (3, N Chetty (3, U Schwingenschlögl (4**

1. University of South Africa, 2. University of Nigeria Nsukka, 3. University of Pretoria South Africa, 4. King Abdullah University of Science and Technology Saudi Arabia

20) Title: **2D Structures of III-VI Materials in Non-Hexagonal Symmetry**

**Jimena Olmos Asar**, Centro de Ciências Naturais e Humanas - UFABC, Santo André, Brazil

21) Title: **Simple Screened Hydrogen Model of Excitons in Two-Dimensional Materials**

**Olsen Thomas**, Technical University of Denmark, Copenhagen, Denmark

22) Title: **Core level binding energies in solids from first-principles**

**Taisuke Ozaki**, Core level binding energies in solids from first-principles, Institute for Solid State Physics (ISSP), The University of Tokyo, Kashiwa, Japan

23) Title: **Lattice dynamics and thermophysical properties of some h.c.p. elements from the quasi-harmonic approximation**

**Mauro Palumbo**, Scuola Internazionale Superiore di Studi Avanzati (SISSA), Trieste, Italy



- 24) Title: **Improvements on non-equilibrium and transport Green function techniques: the next-generation transiesta**  
**Nick Papior**, INSTITUT CATALÀ DE NANOCIÈNCIA I NANOTECNOLOGIA, Bellaterra, Barcelona, Spain
- 25) Title: **A DFT study of band gap of few layers phosphorene applying in-plane strains**  
**Mansoureh Pashangpour**, Islamic Azad University - Islamshahr Branch, Science, Department, Tehran, Iran
- 26) Title: **Periodic lattice distortion and electronic structure of monolayer rhenium disulphide ReS<sub>2</sub>**  
**Diego Pasquier**, EPFL - School of Basic Sciences, Institute of Physics, Chairs of computational condensed matter physics, Lausanne, Switzerland
- 27) Title: **Electronic Structure Evolution during the Growth of Graphene Nanoribbons on Au(110)**  
**Claudia Maria Pereira Cardoso**, S3 Center, Istituto Nanoscienze CNR, Modena, Italy
- 28) Title: **ENHANCEMENT OF ELECTRON-PHONON COUPLING IN ALKALI-DOPED GRAPHENE AND THIN MgB<sub>2</sub> LAYERS**  
**Jelena Pešić, Igor Popov, Vladimir Damjanović, Radoš Gajić**, Graphene Laboratory, Center for Solid State Physics and New Materials, Institute of Physics, University of Belgrade, Belgrade, Serbia
- 29) Title: **The effect of strain on Ag<sup>+</sup> cation substitution in CdSe nanocrystals**  
**Urko Petralanda**, Italian Institute of Technology, Genoa, Italy
- 30) Title: **Exploring point defects in the 1T' phase of single-layer MoS<sub>2</sub>**  
**Michele Pizzochero**, Chair of Computational Condensed Matter Physics, Institute of Physics École Polytechnique Fédérale de Lausanne (EPFL), Lausanne, Switzerland
- 31) Title: **Origin of surprising attractive lateral interactions between oxygen adatoms on aluminum surfaces**  
**Matic Poberžnik**, Department of Physical and Organic Chemistry, "Jožef Stefan" Institute, Ljubljana, Slovenia
- 32) Title: **The EPW code**  
**Samuel Ponce**, Université catholique de Louvain, Louvain-la-Neuve, Belgium
- 33) Title: **An Investigation of Group V dopants in Silicon using Linear Scaling DFT**  
**Jack Poulton**, London Centre for Nanotechnology, London, United Kingdom
- 34) Title: **Is DFT photorealistic for precious metals?**  
**Gianluca Prandini**, École polytechnique fédérale de Lausanne, EPFL, STI IMX THEOS Lausanne, Switzerland
- 35) Title: **First-principles anharmonic calculations and the dynamic Jahn-Teller effect**  
**Joseph Prentice**, TCM Group, Cavendish Laboratory, University of Cambridge, Cambridge, United Kingdom
- 36) Title: **Magnetic susceptibility and magnetoelectric monopolization from density functional perturbation theory**  
**Sergei Prokhorenko**, Theoretical Materials Physics, Université de Liège, Sart Tilman, Liège, Belgium



37) Title: **Fundamental role of defect diffusion barriers and temperature on RRAM switching mechanism**

**Federico Raffone**, Politecnico di Torino, Dipartimento di Scienza Applicata e Tecnologia, Torino, Italy

38) Title: **Dynamic Covalent Bond from First Principles: Diarylbibenzofuranone Antioxidant Properties, Molecular and Electronic Structure**

**Gabriel Ravanhani Schleder**, Federal University of ABC, Santo André, Brazil

39) Title: **Non-collinear magnetism in the Abinit Density Functional Perturbation Theory**

**Fabio Ricci**, Physique Théorique des Matériaux, University of Liège, Liège, Belgium

40) Title: **Graphene based materials as novel membranes for water desalination and boric acid separation**

**Francesca Risplendi**, Politecnico of Turin, Applied Science and Technology Department, Turin, Italy

41) Title: **NEW ADVANCEMENTS IN THE STUDY OF THE UNIFORM ELECTRON GAS WITH FULL CONFIGURATION INTERACTION QUANTUM MONTE CARLO**

**Michele Ruggeri**, Max Planck Institute for Solid State Research, Stuttgart, Germany

42) Title: **Approximate Exchange Kernel RPA for the Condensed Phase**

**Vladimir Rybkin**, University of Zurich, Zurich, Switzerland

43) Title: **An ab initio investigation of the structural and electronic properties of Graphene Oxide**

**Filippo Savazzi**, DISAT, Politecnico di Torino, Torino, Italy

44) Title: **Many-body perturbation theory - the Sternheimer-GW method**

**Martin Schlipf**, Department of Materials, University of Oxford, Oxford, United Kingdom

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**Patrick Seewald**, University of Zurich, Department of Chemistry, Zurich, Switzerland

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**Jonathan Skone**, Univ. of Chicago, Institute for Molecular Engineering, Eckhardt Research Center

47) Title: **DFT-MD study of superconcentrated Li-salt electrolytes for Lithium-ion batteries**

**Keitaro Sodeyama**, National Institute for Materials Science (NIMS), Center for Materials Research by Information Integration (cMI2), Tsukuba, Japan

48) Title: **Long-wavelength optical phonons in two-dimensional polar materials**

**Thibault Sohler**, THEOS and MARVEL, École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland

49) Title: **DensToolKit: A comprehensive open-source package for analyzing the electron density and its derivative scalar and vector fields. Current developments.**

**Juan Manuel Solano Altamirano**, Faculty of Chemistry, Meritorious Autonomous University of Puebla, Puebla, Mexico



- 50) Title: **Electronic Properties of Organometallic Graphyne Networks on Ag(111)**  
**Himadriben R. Soni**, Lehrstuhl fuer Theoretische Chemie, Friedrich-Alexander Universitaet Erlangen-Nuernberg, Erlangen, Germany
- 51) Title: **Planar versus three-dimensional growth of metal nanostructures at graphene**  
**Srdjan Stavrlic**, Univ. of Belgrade, Vinca Institute of Nuclear Sciences, Laboratory for Theoretical and Condensed Matter Physics, Belgrade, Serbia
- 52) Title: **Tunable quantum conductance in MoS<sub>2</sub> nanoribbons**  
**Fateme Tabatabaei**, Department of Physics, Isfahan University of Technology, Isfahan, Iran
- 53) Title: **Effects of dopants different configurations on electronic structure and magnetic properties of N-doped graphene: an ab-initio study**  
**Yavar Taghipour Azar**, Theoretical and Computational Physics Group, Physics and accelerator school Atomic Energy Organization of Iran, AEOI, Teran, Iran
- 54) Title: **Graphene trumpets, foams, pillared networks, carbon materials growth, and all that from first-principles and classical molecular dynamics simulations**  
**Simone Taioli**, European Centre for Theoretical Studies in Nuclear Physics and Related Areas, Trento, Italy
- 55) Title: **ZnO Nanoporous: Structural and Electronic Study Under Elastic Strain**  
**Alvaro David Torrez Baptista**, Universidade Federal do ABC, Santo André, Brazil
- 56) Title: **High-Throughput Generation and Analysis of a Large Dataset of Organic/Inorganic Hybrid Perovskites**  
**Huan Tran**, Institute of Materials Science, University of Connecticut, Storrs, USA
- 57) Title: **First-principles calculation on rare earth doped tellurides: thermoelectric and magnetic properties**  
**Van Quang Tran**, Department of Physics, University of Transport and Communications Hanoi, Vietnam
- 58) Title: **Probing the electronic structure for 3d-3p and 3d-3s hybridized states using resonance photo-emission spectroscopy**  
**Malvika Tripathi**, Thin Film Magnetism (SVSM) and PLD Lab., UGC DAE Consortium of Research, Indore, India
- 59) Title: **Current-induced orbital magnetism in doped tellurium.**  
**Stepan S. Tsirkin, Pablo Aguado, Ivo Souza**, University of the Basque Country, San Sebastian, Spain
- 60) Title: **First-Principles Study of The Electronic Structure in Molecular Conductors with Hybrid Functional**  
**Takao Tsumuraya**, International Center for Young Scientists, National Institute for Materials Science, Tsukuba, Japan
- 61) Title: **Delivering on the promises of high-throughput atomistic simulations using verification, data provenance and workflows**  
**Martin Uhrin**, École Polytechnique Fédérale de , Lausanne, Switzerland
- 62) Title: **Anisotropic thermal conductivity of arsenene and phosphorene: An ab initio study**  
**Syedmehdi Vaezallaei**, Department of Physics, University of Tehran, Tehran, Iran



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**Daniele Varsano**, CNR, Institute of Nanoscience, Modena, Italy

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**George Yumnam**, Materials Research Centre, , Indian Institute of Science, Bangalore , Faculty: Prof. Abhishek Kumar Singh, Bangalore, India

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