

POSTER SESSION II

FRIDAY, JANUARY 13, 2017

18:00, Adriatico Guesthouse, Lower Level

M - Z in alphabetical order by Author (REVISED - see names at bottom)

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 Sb₂Te₃**

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_xCo_{1-x} 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 Ti₃C₂MXene**

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

9) Title: **First Principle study of CO₂ adsorption on TiO₂ 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 Nagney, 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 ReS₂**
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 MgB₂ 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⁺ 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 MoS₂**
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

45) Title: **Analytical integrals for fast electron correlation of periodic systems**

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

46) Title: **Dielectric-dependent Hybrid Functionals for Accurate Electronic Structure of Molecules and Periodic Systems**

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 Stavric, Univ. of Belgrade, Vinca Institute of Nuclear Sciences, Laboratory for Theoretical and Condensed Matter Physics, Belgrade, Serbia
- 52) Title: **Tunable quantum conductance in MoS₂ nanoribbons**
Fatemeh tabaei, 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**
Seyedmehdi Vaezallaei, Department of Physics, University of Tehran, Tehran, Iran

63) Title: **Modeling the FePc adsorption on the moire superstructure of graphene intercalated with a Co layer**

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

64) Title: **Nanotherm: Ab initio integrated tool to describe thermoelectricity {in nanostructures from materials to devices**

Nathalie M.M. Vast, Laboratoire des Solides Irradiés Ecole Polytechnique) CEA/DSM/IRAMIS / CNRS UMR7643, Palaiseau, France

65) Title: **Encapsulated Nanowires: Boosting Electronic Transport in Carbon Nanotubes**

Andrij Vasylenko, Department of Physics, University of Warwick, Coventry, United Kingdom

66) Title: **Invisible Gold Adatoms and where to find them: the case of Dimethyl Sulfoxide on a Gold Surface**

Simone Velari, Università degli Studi di Trieste, Trieste, Italy

67) Title: **Cubic scaling RPA correlation energy calculations**

Jan Wilhelm, University of Zurich, Department of Chemistry, Zurich, Switzerland

68) Title: **Oxygen reduction reaction on the defective tetragonal ZrO₂(101) surface**

Yoshiyuki Yamamoto, The Institute for Solid State Physics, The University of Tokyo, Kashiwa, Japan

69) Title: **Optical fingerprints of solid-liquid interfaces: a joint ATIR and first principles investigation**

Lei Yang, Max-Planck-Institut fuer Eisenforschung GmbH, Dusseldorf, Germany

70) Title: **High temperature thermoelectric study on Zr and Hf based transition metal dichalcogenides**

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

71) Title: **Temperature effects on the relative stability of ultra-high pressure phases of oxygen**

Beatriz Helena Cogollo Olivo, Universidad de Cartagena, Campus San Agustin, Programa de Doctorado en Ciencias Fisicas, Tercer Piso, Cartagena De Indias, Colombia

NEW ENTRIES:

72) Title: **Simulations of water nano-confined between corrugated planes**

Emilio Artacho, Theory of Condensed Matter, Department of Physics, Cavendish Laboratory, University of Cambridge, Cambridge, UK

73) Title: **GW calculations of anatase TiO₂ systems of different dimensionality**

Ivan Marri, S3 Center, Istituto Nanoscienze, CNRnano, Modena, Italy

74) Title: **The microscopic dynamics of ABO₃ perovskites**

Giovani Pizzi, (THEOS), (MARVEL), École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland

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

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

76) Title: **Charge localization and energetics of Li-ion batteries cathodes from extended Hubbard-corrected functionals**

Matteo Cococcioni, Ecole Polytechnique Federale de Lausanne, EPFL, Lausanne, Switzerland

77) Title: **Hubbard interactions from density-functional perturbation theory**

Iurii Timrov, Swiss Federal Institute of Technology Lausanne (EPFL)

Laboratory of Theory and Simulation of Materials (THEOS), Lausanne, Switzerland

78) Title: **Simulations of electron energy loss spectra with turboEELS: preliminary results**

Oleksandr Motornyi, Michèle Raynaud and Nathalie Vast, Laboratoire des Solides Irradiés, Ecole Polytechnique - CEA/DRF - CNRS UMR 7642, 91128 Palaiseau cédex, France