

POSTER SESSION I
(revised Jan 12, 2017)
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.Valencia¹ and M.J.Caldas¹, ¹Institute 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 Ni₃TeO₆ 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 Aseguinolaza Aguirreche, Material Physics Center (MPC), San Sebastian, Spain

7) Title: **Electronic and Optical properties of hydrogenated TiO₂**

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

8) Title: **First Principle Calculations of LiRh₂Ge and LiCu₂Ge Heusler Alloys**

Seyfettin Ayhan, Graduate School of Natural and Applied Science, Diyarbakır, 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 In₂Te₃ compound**

Marco Bernasconi, Università 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-YMnO₃**

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 Física 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, Università 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 MoS₂ monolayer**

Giancarlo Cicero, Politecnico di Torino, Torino, Italy

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

Nicola Colonna, Ecole Polytechnique fédérale de Lausanne (EPFL), Lausanne, Switzerland

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

Francesca Costanzo, Catalan 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 α -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)₂Se₃ 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 CaF₂ 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 TiSe₂ 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 Adegboyege 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/SiO₂ 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 WS₂ semiconductor**
Hamideh Kahnouji, Isfahan University Of Technology, Department of Physics, Isfahan, Iran

53) Title: **DFT study of fundamental properties of α' -Fe₁₆C₂ 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: **Microfaceting of Cu₂O and its implications in photochemistry**
Yunjae Lee, Global E3 Institute and Department of Materials Science and Engineering, Yonsei University, Seoul, Korea

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

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

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