Inauguration of the academic year 2016/2017
Department of Chemistry

November 21, 2016

Aula Magna

Via Giuria 7, - 10125 Torino, Italy

Symposium Honoring Prof. Roberto Orlando

Theoretical Chemistry Group, Università degli Studi di Torino

Prof. Roberto Orlando

Our dear friend and colleague Roberto Orlando passed away prematurely, after a long and courageous battle against cancer, on April 19, 2016.

Born in 1961, he graduated in Chemistry in 1986 at the University of Torino. His career started in the Theoretical Chemistry Group of the University of Torino. From 1997 to 2012, he was faculty researcher at the University of Eastern Piedmont. In 2012, he came back at the University of Torino, where he was associate professor in Physical Chemistry since 2014.

Since his M.Sc. degree, Roberto has been developing and applying theoretical quantum mechanical methods for the ab initio study of the electronic structure of solids. He was one of the main developers of the CRYSTAL code. His contribution in this respect has been invaluable. He organized and was a speaker at numerous international schools on ab initio modelling of solids over the years. His passion for research and teaching was recognized by his international colleagues and students.

Besides being an excellent scientist, Roberto has always been a sweet and caring person.

Program

Monday – November 21, 2016

Aula Magna di Chimica, Via Giuria 7

9.00 AM	**Prof. Marco Vincenti,** Director of the Department of Chemistry ***"Introductory Remarks"***
9.10 AM	**Prof. Roberto Dovesi,** University of Torino ***"Roberto Orlando: a life in quantum mechanical simulation"***
Invited lectures	***Session Chair: Prof. Piero Ugliengo,*** *University of Torino*
9.25 AM	**Prof. Victor Luana,** University of Oviedo, Oviedo, Spain ***"How thermodynamic properties of crystals can de predicted at the temperatures and pressures at 500 km under our feet"***
10.05 AM	**Dr. Kah Chun Lau**, California State University Northridge, Northridge, USA ***"Atomistic Simulation of Alkali-Metal (Li, Na) based Electrical Energy Storage"***
10.45 AM	***Coffee Break***
11.15 AM	**Prof. Ravindra Pandey,** Michigan Technological University, Houghton, MI USA ***"Phosphorene-based 2D materials"***
11.55 AM	**Padre Antonio Marangon,** Responsabile comunità di accoglienza Madian per ammalati stranieri, Torino ***" Roberto Orlando e il volontariato"***

Invited Lectures

Abstracts

How thermodynamic properties of crystals can de predicted at the temperatures and pressures at 500 km under our feet

Victor Luaña (1) and Alberto Otero-de-la-Roza (2)

(1) Departamento de Química Física y Analítica, Universidad de Oviedo, Oviedo, Spain
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(2) Department of Chemistry, University of British Columbia Okanagan, Canada

Theoretical calculation of thermodynamic properties is nowadays possible within the context of the quasi-harmonic approximation. In this talk I will try to embark into a journey into the mathematical and computational road that led us to the elastic behavior of crystalline materials with unprecedented accuracy. DFT in the Kohn-Sham formalism created a revolution in theoretical chemistry, but the perfect functional is being slowly developed. In the meantime I will show that thermodynamic properties can be obtained within experimental accuracy using current approximate density functionals. Even though the purpose of theoretical work is not substituting experiments, predictability is required as the number of chemicals and materials grows faster than the capabilities to determine its properties precisely.

Atomistic Simulation of Alkali-Metal (Li, Na) based Electrical Energy Storage

Kah Chun Lau

Department of Physics, California State University Northridge, Northridge, CA, USA
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"Energy" is an important concept in physics. More importantly, electric energy is extremely crucial in our daily lives in many applications. The ever increasing need for electricity will require foremost increased efficiency in the uses of electric energy, more secure and diversified energy resources, and a successful strategy to tame greenhouse gas emissions around the globe. To get it right, it is deemed necessary to turn into "sustainable" renewable energy resources (e.g. solar, wind, etc.) for future energy consumption, to fix our current energy problems. Unfortunately, solar and wind energy are intermittent, whereas the electricity that we need must be reliably available for 24 hours a day with minimal second-to-

second fluctuations. To be better tailored to these challenges, electrical energy storages (e.g. batteries) that can efficiently store and deliver electric energy will therefore be critical for effectively leveling the cyclic nature of renewable energy resources. To accelerate fundamental research in this new field, computational modeling especially the atomistic simulation in chemistry and materials science can provide accurate and timely solutions. In this symposium, I will share with you some of my thoughts and our recent works in alkali-metal (e.g. Li, Na) batteries using molecular dynamics and first principles methods.

Phosphorene-based 2D materials

Ravindra Pandey

Department of Physics, Michigan technological University, Houghton, MI, USA
(pandey@mtu.edu)

Phosphorene, the monolayer form of the (black) phosphorus, was recently exfoliated from its bulk counterpart. Phosphorene oxide, by analogy to graphene oxide, is expected to have novel chemical and electronic properties, and may provide an alternative route to synthesis of phosphorene. In this talk, we will report the results of density functional theory calculations on phosphorene-based 2D materials including hybrid allotropes of phosphorene and phosphorene oxide. We will show that the oxygen absorption may not degrade the phosphorene, and degree of the functionalization of phosphorene determines the electronic properties. This is reaffirmed by dependence of the diode-like asymmetric current-voltage response on the degree of stoichiometry for the phosphorene oxide.

Invited Lectures

Lecturer's short biographies

Prof. Victor Luaña

Victor Luaña was born in Oviedo, on a February 29-th of 1960. He went to the colegio Loyola, of the Escolapios Fathers and to the IES Alfonso II for the primary and secondary studies. Then he obtained a Chemistry degree with honors in the Universidad de Oviedo, obtaining the Prize «Química del Nalón» and «Extraordinario de Licenciatura» as the best student in the class. A grant, «Formación de Personal Investigador», from the Ministry of Education allowed him to continue his formation, starting to work in the research group founded by Lorenzo Pueyo. He did a Master Thesis, «Estudio de las interacciones core-valencia en el cálculo de la estructura electrónica de átomos e iones según el método del potencial modelo», under the main advise of Zoila Barandiarán, and completed a PhD degree under the direction of Lorenzo Pueyo. His PhD Thesis «Aplicación de la Teoría de la Separabilidad Electrónica al estudio de la estructura electrónica y propiedades de los iones de transición 3d en cristales iónicos», provided him the prizes "Extraordinario de Doctorado" and "San Alberto Magno" (this one with a nice allowance included). A short period as computer science teacher provided him the stability and resources to marry, at last, Margarita in 1997, my girlfriend since we both were undergrads. He went then, thanks to a Fulbright grant, to the Department of Chemistry of the Ohio State University in Columbus OH, to collaborate as a postdoc in the research group of Russell M. Pitzer. The economic and academic situation in Spain improved so much with respect to previous years that he decided to renounce to the continuation of his grant. Back in Oviedo, He occupied several positions until obtaining a permanent position as a «Titular de Universidad», and acted as manager of new vectorial computer. Shortly after that, Barcelona and Sevilla organized worldwide meetings to celebrate that his beloved daughter Andrea Victoria was finally born :). I could say, after all, that I have a special relationship with leap years.

Dr. Kah Chun Lau

Dr. Kah Chun Lau is currently an Assistant Professor at Department of Physics and Astronomy from California State University Northridge (CSUN) at California, USA. Before joining CSUN, he was an Assistant Physicist at Materials Science Division of Argonne National Laboratory, Illinois. After recieving his Ph.D. in physics (2007) from Michigan Technological University, he worked a postdoctoral researcher at U.S. Naval Research Laboratory (2007-2009) and Argonne National Laboratory (2010-2013). He has published nearly 60 peer-reviewed publications and his current

research interest is in fundamental study of Li-ion and beyond Li-ion batteries (e.g. metal-O2 battery, Li-S battery) based on multiscale atomistic simulation.

Prof. Ravindra Pandey

Ravindra Pandey is Professor and Chair of Physics at the Michigan Technological University, Houghton, MI. Pandey received his education at Hari Singh Gaur University, Sagar, National Physical Laboratory, Delhi, Atomic Energy Research Laboratory, Harwell, UK and University of Manitoba, Winnipeg, Canada. He has participated in multi-disciplinary efforts (theoretical and experimental) to build the programs in novel nanostructures, and application of chalcopyrite semiconductors as the next generation optoelectronic materials with the industrial and national laboratories, and is the author of more than 150 publications. He has also co-organized and participated in several international conferences in the areas of Materials Physics and Nanoscale Science. Pandey is Fellow of American Physical Society