

ESCUELA POLITÉCNICA NACIONAL

DEPARTAMENTO DE FÍSICA

XVII PHYSICS MEETING



October 2021

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WELCOME

Dear participants,

On behalf of the organizing committee, I would like to express our gratitude for sharing and discussing the results of your actual research in the framework of the XVII Encuentro de Física.

We are convinced these venues to enhance and foster the possibilities to establish and strengthen working and friendship networks, are also the place where new ideas and projects begin, and finally, play a key role in motivating young researchers and students. This is particularly true in our Country, where such occasions are normally scarce. The Encuentro de Física has already established itself as a much-valued and expected tradition in this respect, and we are proud of having had the opportunity in this difficult year of maintaining its relevance and quality. In a great measure, this is due to your participation.

The pandemic caused by COVID-19 forced, unfortunately, to change the usual format of our conference into a virtual one. But on the other hand, this also provided obvious advantages. One of these advantages is that we could welcome the participation of 13 outstanding keynote speakers, who are well-known leaders in their fields without having to incur greater logistic problems. Additionally, it was possible to receive contributions from researchers working in several countries of Latin America and Europe, who could participate without the need of securing funds for traveling, which could represent a problem.

As mentioned, the program includes 13 keynote speakers, 52 oral, and 26 poster contributions. Prior to the conference, we have organized five practical workshops on mechanics, electromagnetism, optics, biophysics, scientific programming, and the teaching of physics. We are pleased to have been able to bring back such hands-on activities to the program.

This event is only possible thanks to the effort of the Professors of the Department of Physics at EPN, and thanks to the committed help of the students, assistants, and administrative personal of the Department and EPN. Of course, without the engagement of the researchers and public, this would neither have been not possible nor would have a purpose. Thank you!

We hope The XVII Encuentro de Física will meet your expectations and wish you a fruitful and interesting conference!

Esteban Iribarra
Chair of the XVII Physics Meeting

HISTORY OF THE ENCUENTRO DE FÍSICA

El Encuentro de Física (The Physics Meeting) is a traditional event organized biennially by the Department of Physics of Escuela Politécnica Nacional (National Polytechnic School). The first edition of this meeting was held in 1989, and since then, every two years a new edition of the meeting has been developed.

The objectives of the Physics Meeting from the beginning have been:

Create a space to disseminate and debate academically the results of the most recent research carried out nationally and internationally in the different areas of study of physics. Establish networks between teachers, students and people interested in physics in Ecuador and the region. Develop workshops, active learning experiences in laboratories to improve the understanding of physics at both secondary and higher education levels. From its beginnings to the present date, 16 editions of the Physics Meeting have been organized and in this way, an open, participatory and integrative space has been built, through the development and generation of a critical and research academic community in the most relevant topics of physics.

Each edition of the event has focused on contemporary areas or research topics in physics. In the most recent editions, the meeting has focused on the Nanoscience Revolution (2009), Nuclear and Radiation Physics and the peaceful use of nuclear energy (2011), The Frontiers of Physics in Latin America (2013), Optics, in the context of the declaration of the International Year of Light by UNESCO (2015), Condensed Matter (2017) and Computational Physics (2019).

To promote the exchange of scientific knowledge for the benefit of students and the academic community in general, we have had the presentation of papers, keynote talks and lectures given by different invited researchers.

In the different editions of the event, the participation of renowned researchers has been counted. Some of the most outstanding national and international researchers who have been part of the different editions of the meeting, presenting lectures, have been: Dr. Pablo Mininni (Argentina, 2019), Prof. Sokrates Pantelides (USA, 2017), Dr. Katja Lindenberg (USA, 2015), Dr. Alexander Kubankin (Russia, 2015), Dr. Silvia Braslavsky (Germany, 2015), Dr. Vanderlei Bagnato (Brazil, 2013), Dr. Ivan Schuller (USA, 2009), among others. There has also been the participation of undergraduate and graduate students from the country and the region, who have participated in poster presentation sessions and conferences with topics related to their degree work.

COMMITTEE

ORGANIZING COMMITTEE

- DR. ESTEBAN IRRIBARRA - Chair
- DRA. ELIANA ACURIO - Co-Chair
- DR. CÉSAR COSTA - Co-Chair

SCIENTIFIC COMMITTEE

- LEONARDO BASILE - ESCUELA POLITÉCNICA NACIONAL (NATIONAL POLYTECHNIC SCHOOL)
- GABRIEL BILMES - UNIVERSIDAD NACIONAL DE LA PLATA (NATIONAL UNIVERSITY OF LA PLATA)
- THOMAS CADENBACH - UNIVERSIDAD SAN FRANCISCO DE QUITO (SAN FRANCISCO UNIVERSITY OF QUITO)
- JOSÉ LUIS PAZ - UNIVERSIDAD NACIONAL DE SAN MARCOS (NATIONAL UNIVERSITY OF SAN MARCOS)
- LUCA SORRISO-VALVO - SWEDISH INSTITUTE OF SPACE PHYSICS, UPPSALA UNIVERSITY

COLLABORATORS

- Fis. Fernando Moncada
- Fis. Cristopher Erazo
- Fis. José Toabanda
- Ing. Janneth Peña
- Ing. Julio Erazo
- Tnlga. Karina Guerrero
- Mgtr. Paola Vega

KEYNOTES

ASTRONOMY

A journey near the sun: first results of the solar orbiter satellite

DR. LUCA SORRISO-VALVO

Biography:

Dr. Luca Sorriso-Valvo studied his bachelor's and Ph.D. in Physics at the University of Calabria: Rende, Italy. His expertise focuses on data analysis and spatial plasma modeling and dynamics of complex systems. The fields that interest him are: turbulence in space plasma, solar physics, non-linear dynamics, space weather. He did his postdoctoral work at the University of Calabria and had a research stay at the University of California, Berkeley. Additionally, he was an associate professor at the National Polytechnic School from 2018 to 2020 and now is working at the Swedish Institute of Space Physics.

Abstract:

On February 10, 2020, a rocket that put the European Space Agency's (ESA) Solar Orbiter satellite into orbit around the sun took off from Cape Canaveral. With each turn, the probe gets closer to the star, so that by this date its perihelion is no longer so far from mercury's orbit. After more than a year and a half, the first measurements of the satellite have been developed, resulting in numerous scientific publications. These include the observation of nanoflares in the solar chromosphere, the observation of the magnetic field and high-energy particles in the magnetosphere of Venus, and a wide variety of waves and turbulent phenomena in the solar wind. In this talk, after a report on the state of the satellite, the most important results obtained will be presented, and the plan of observations expected in the coming years will be reviewed.

HIGH ENERGY PHYSICS

DARK MATTER AND STANDARD MODEL

DR. BRUCE HOENEISEN

Biography:

Bruce Hoeneisen obtained his PhD in Electrical engineering and Physics (1972) and his master's degree in Electrical Engineering (1970) at the California Institute of Technology while his undergraduate degree in civil and electrical engineering was obtained at the University of Chile (1968). He was a professor in physics at the EPN from 1972 to 1986, an independent consulting engineer in Quito since 1978, director of applied sciences at the Universidad San Francisco de Quito since 1988. He has been listed as a notable physicist in "Marquis Who's Who".

Abstract:

84% of the matter in the universe is "Dark Matter" of unknown origin. I present detailed measurements of the properties of Dark Matter by studying rotation curves of spiral galaxies, and independently, of the distributions of stellar masses of galaxies.

ELECTROWEAK INTERACTIONS: FROM DISCOVERY TO PRECISION TESTS OF THE STANDARD MODEL

DR. MAARTEN BOONEKAMP

Biography:

Maarten Boonekamp, Ph.D. es director de investigación en el Instituto de Investigación de las Leyes Fundamentales del Universo, IRFU, CEA. Obtuvo su licenciatura en Física Fundamental (1995) y su doctorado en DAPNIA / SPP y Universidad de París VII (1999). Es miembro de los experimentos DELPHI y ATLAS, especializado en Higgs y Física Electrodébil con más de 1000 publicaciones, de las cuales más de 50 contienen contribuciones personales importantes o destacadas. Además, es experto en calibración de electrones y fotones en ATLAS, con el objetivo de realizar mediciones precisas de parámetros fundamentales electrodébiles, en particular las masas del bosón W y de Higgs, y el ángulo de mezcla débil efectivo. En su investigación personal (producción de bosón de Higgs en eventos difractivos, interacciones fuertes, metodología de medición de parámetros electrodébiles) cuenta con 35 publicaciones (autor principal) y dos artículos de revisión invitados. De 2001 a 2003 fue investigadora en el CERN (Ginebra). En 2015 ganó el premio Joliot-Curie de la Sociedad Francesa de Física. Y obtuvo una beca de investigación de la ANR ("Agence Nationale de la Recherche") sobre física electrodébil en el LHC.

Abstract:

Through a brief historical introduction to the Drell-Yan process and the discovery of the electroweak gauge bosons, It will be summarized how the measurements of their production and decay properties allow to test such different things as the structure of the proton and the electroweak theory, and the guidance this provides in searches for yet undiscovered particles.

MACHINE LEARNING / COMPLEX SYSTEMS

ARTIFICIAL INTELLIGENCE FROM PHYSICS

DR. KONRAD KORDING

Biography:

Konrad Paul Kording, Ph.D. is a professor at the University of Pennsylvania. He obtained his undergraduate degree (1997) and PhD (2001) in physics at the Federal Polytechnic School in Zurich. He has completed post-doctoral stays at the Swiss College of Zurich and University College of London where he obtained a Position of Heisenberg Fellow at MIT. In 2017 he joined the Department of Neuroscience and also the Department of Bioengineering at the University of Pennsylvania. Currently his research work is focused on methods of neural data analysis and methods of obtaining large sets of neural data.

Abstract:

Machine learning is starting to be a workhorse of science, engineering, and society. We use it for everything from cosmology, via self-driving cars, to deciding who gets a credit card. And yet, we are still limited at understanding why the various machine learning approaches even work. In my talk I will review how machine learning is relevant across society. I will also discuss various ways from physics and mathematics for understanding how learning works. Lastly, I will argue for more integration between all these field.

COMPLEX NETWORKS AND THEIR APPLICATIONS

DR. VITALY BELIK

Biography:

Dr. Vital Belik is an assistant professor at the Institute for Veterinary Epidemiology and Biostatistics at Free University of Berlin, and he is leader of Working Group System Modelling. He obtained his diploma (with honors) in Physics and Biochemical Physics (2004) from Lomonosov Moscow State University, PhD in Theoretical Physics from Georg-August-Universität Göttingen (2008) and postdoctoral experience at Massachusetts Institute of Technology (2012). He has worked as consultant intern at D-Fine, researcher at Max Planck Institute for Dynamics and Selforganization, visiting scientist at Helmholtz center for Infection Research and as research associate at Institute for Theoretical Physics, Technische Universität Berlin. His research focuses on Microbiome dynamics, Computer vision and Machine learning in animal health applications, Disease spread on networks of hospitals and animal trade networks, Time series analysis in application to sensor data on animal behavior for health monitoring, Parasite-host-environment dynamics and Hormon dynamics in dogs. Also, he is Co-Organizer of the Berlin Colloquium Statistical Methods in Empiric Research, Representative of FU Berlin in Data Literacy Education Network of

Stifterverband and Review Editor on the Editorial Board of Frontiers in Veterinary Science COST Action Workshop organizer (Networks in One Health Epidemiology)

Abstract:

Complex networks is a vivid field of research having its roots in mathematical graph theory originating at least in the 18th century. Nowadays networks represent a suitable framework predestined for description of complex systems in a large range of spatial and temporal scales – from molecular (e.g. protein-protein interaction networks) to societal (e.g. contact networks) and planetary scale (e.g. transportation networks). Complex system are consisting of many individual units (nodes or vertices) interacting with each other. Interactions are described as edges or links between vertices. In this talk I will provide an introduction into network science and its applications especially in the field of epidemiology.

MEDICAL PHYSICS

ARTIFICIAL INTELLIGENCE IN MULTIMODALITY MEDICAL IMAGING: PAST, PRESENT, ANY FUTURE?

DR. HABIB ZAIDI

Biography:

Professor Habib Zaidi is head of the PET Instrumentation & Neuroimaging Laboratory at Geneva University Hospital and faculty member at the medical school of Geneva University. He is also a Professor of Medical Physics at the University of Groningen (Netherlands), Adjunct Professor of Medical Physics and Molecular Imaging at the University of Southern Denmark, Adjunct Professor of Medical Physics at Shahid Beheshti University and visiting Professor at Tehran University of Medical Sciences. He is actively involved in developing imaging solutions for cutting-edge interdisciplinary biomedical research and clinical diagnosis in addition to lecturing undergraduate and postgraduate courses on medical physics and medical imaging. Prof. Zaidi has been an invited speaker of over 160 keynote lectures and talks at an International level, has authored over 700+ publications including 323 peer-reviewed journal articles in prominent journals, 340 conference proceedings and 41 book chapters. His academic accomplishments in the area of quantitative PET imaging have been well recognized by his peers and by the medical imaging community at large since he is a recipient of many awards and distinctions.

Abstract:

This talk presents the fundamental principles and major applications of artificial intelligence (AI), in particular deep learning approaches, in multimodality medical imaging. To this end, the applications of deep learning in five generic fields of multimodality medical imaging, including imaging instrumentation design, image denoising (low-dose imaging), image reconstruction, quantification and segmentation, radiation dosimetry and computer-aided diagnosis and outcome prediction are discussed. Deep learning algorithms have been widely utilized in various medical image analysis problems owing to the promising results achieved in image reconstruction, segmentation, regression, denoising (low-dose scanning) and radiomics analysis. This talk reflects the tremendous increase in interest in quantitative molecular imaging using deep learning techniques in the past decade to improve image quality and to obtain quantitatively accurate data from dedicated combined PET/CT and PET/MR systems. The deployment of AI-based methods when exposed to a different test dataset requires ensuring that the developed model has sufficient generalizability. This is an important part of quality control measures prior to implementation in the clinic. Novel deep learning techniques are revolutionizing clinical practice and are now offering unique capabilities to the clinical medical imaging community. Future opportunities, the challenges facing the adoption of deep learning approaches and their role in molecular imaging research are also addressed.

GEL DOSIMETRY, APPLICATIONS OF MACHINE LEARNING IN RADIOTHERAPY

DRA. JULIANA PAVONI

Biography:

Juliana Pavoni is an assistant professor at the Department of Physics, Faculty of Philosophy, Science and Letters of Ribeirão Preto - University of São Paulo and works as a clinical medical physicist in radiotherapy at the Ribeirão Preto Medical School Hospital and Clinics - University of São Paulo. She received a BS degree in medical physics (2004) and a Ph.D. degree in Physics Applied to Medicine and Biology (2009) from the University of São Paulo. She has experience in Medical Physics, with a particular interest in radiopharmacy quality control tools, including gel dosimetry and artificial intelligence.

Abstract:

The use of machine learning and other sophisticated models to aid in prediction and decision-making has become widely popular across the medical field. The situation is not different in radiotherapy. These resources allow automation and workflow optimizations, especially in automatic segmentation, planning, and quality assurance. In this presentation, an overview of the application of these tools in radiotherapy will be discussed.

OPTICS

LOW-COST METHODS AND INSTRUMENTS FOR ADVANCED HOLOGRAPHIC MICROSCOPY

DR. AYDOGAN OZCAN

Biography:

Dr. Aydogan Ozcan received his Ph.D. degree from the Department of Electrical Engineering at Stanford University. He joined UCLA in 2007 and is currently Chancellor Professor and HHMI Professor at the Howard Hughes Medical Institute. He holds more than 45 registered patents (and more than 20 in process) for his inventions in telemedicine, mobile health, nonlinear optics, optical fibers, optical coherence tomography, etc. He has given more than 70 plenary lectures and more than 350 invited talks. He is the author of a book and co-author of more than 700 peer-reviewed publications in major journals and conferences. He has received numerous awards, most notably in 2011 when he received the Presidential Young Career Award for Scientists and Engineers (PECASE), which is the highest honor awarded by the U.S. government in science and engineering professionals in early stages of their research careers.

Abstract:

We will discuss diffractive optical networks that can all-optically implement various complex functions, as the input light diffracts through spatially-engineered surfaces. These diffractive processors will find applications in all-optical image analysis, feature detection and object classification, also enabling task-specific camera designs and new optical components.

TEACHING OF PHYSICS

TEACHING OF PHYSICS

DR. ERIC BURKHOLDER

Biography:

Eric Burkholder is an assistant professor of physics at Auburn University in the United States. He runs a research group studying a wide range of phenomena in physics and engineering education including real-world problem solving, student perceptions of physics tasks, student motivation, social psychological factors, and group work. He previously completed a postdoctoral stay in Physical Education at Stanford University under the direction of Nobel Laureate Carl Wieman. He holds a Ph.D. in Soft Matter Physics from the California Institute of Technology and an undergraduate degree in Chemical Engineering from Cornell University.

Abstract:

Traditional university education has remained largely unchanged since medieval times – a professor standing in front of their students telling the students the information they are supposed to learn. Over the past few decades, research has consistently demonstrated that this is a poor method of teaching because it does not actively engage students in the learning process. “Active learning” – any method of teaching in which students are engaged by solving problems, talking to each other, answering conceptual questions, etc. instead of listening to the teacher – has been shown to help students learn new content, decrease failure rates, and improve student’s perceptions of science. There are many different ways of making a classroom more active, but all methods are based on fundamental principles of learning that have been investigated by cognitive scientists. In this talk, I will give a brief overview of the most important principles of learning and discuss practical ways to implement this in the physics classroom. As we go, I will present data showing how these novel methods lead to improved student outcomes. At the end of the talk, I will discuss what factors are necessary to facilitate systemic change in physics teaching. Hopefully, this will inspire individual faculty to adopt more effective teaching practices and encourage administrators to rethink the way teaching is evaluated and valued at the university.

TEACHING OF PHYSICS

DRA. DIANA LÓPEZ TAVARES

Biography:

Diana López obtained her PhD in Physics Education Research from the National Polytechnic Institute of Mexico. She has a master’s degree in Physics Education Research and an undergraduate degree in Physics. He has collaborated with PhET since 2017 working on the design of physics simulations and teaching professional

design to Hispanic professors. Her research focuses on advanced learning in Science, Technology, Engineering and Mathematics (STEM) for students in Latin America and the world using equitable education of the highest quality, supporting programs for the professional development of teachers and designing contextualized study material. She currently works as a Latin American specialist in the PhET project and during the pandemic has focused on the design and implementation of massive virtual courses and virtual teaching activities to enhance remote classes of science teachers.

Abstract:

The PhET project from the University of Colorado Boulder creates interactive simulations and free virtual labs for science and math learning. PhET simulations are used globally, and due to the COVID-19 pandemic, in some regions of the world their use increased by up to 700%, being one of the main resources used by science teachers. It is almost 20 years of the PhET Project and in this conference we will review some of the research results on the impact on student learning and motivation when using simulations in class, the research that is still open in PhET, and the projects that are held in Latin America with the PhET-Global initiative.

LOW-COST EXPERIMENTAL RESOURCES IN THE TEACHING OF PHYSICS TO SHARE WITH TEACHERS

DR. JOSÉ BENITO VÁZQUEZ DORRÍO

Biography:

José Vázquez obtained a degree in Physical Sciences from the University of Santiago de Compostela in 1990 and a PhD in Physics from the University of Vigo in 1996. He has been awarded four six-year periods of CNEAI research and his research in the Engineering Physics Group focuses on applied optics, photonics, and laser technologies. He is co-author of more than 70 publications indexed in SCOPUS, plus 50 publications in congresses and has collaborated in the organization of 14 scientific meetings. He maintains a line of educational innovation in the field of experimental science teaching since 1991 with 10 innovation and scientific transfer projects, 120 publications and 38 participations in the organization of scientific meetings. He currently directs a doctoral thesis, is a regular censor of 5 international journals and is vice president of the Hands-on Science Association. In addition, he is Ambassador for Spain of Scientix and head of the Teaching Innovation Group of Manipulative Learning of Physics.

Abstract:

Almost all reports on education, learning, dissemination, and vocation in the teaching of physics indicate that it is necessary to establish links between the contents of formal learning and the experiential learning inherent in the scientific method. An obstacle that appears when it is intended to carry out this necessary connection lies

in the tendency of teachers to replicate in the classroom the teaching that they have received during their student stage. This teaching often focuses on the theoretical foundations and moves away, in most situations, from an active, practical, and experimental vision. The ability to teach using manipulative, practical, experimental, and material-focused activities should be an objective of the training of teachers who should be offered the possibility of developing competences in this field.

This talk presents an updated review of the possible resources that, in this constructivist context, teachers can use. Different possibilities of use outside and inside the classroom are analyzed, as well as recent results of various training courses carried out for teachers with this methodology. The purpose of the course is to provide participants with an overview of the advantages and possibilities of using experimental activities in formal education, inducing, if possible, their use in their daily teaching work, so that students can "do" science rather than simply being "exposed" to it.

SOLID STATE

PEROVSKITE SOLAR CELLS

DR. WOLFGANG TRESS

Biography:

Dr. Wolfgang Tress is currently a full professor at the University of Applied Sciences in Zurich. He studied at the Technical University of Dresden. He is the author of the renowned book “Organic Solar Cells: Theory, Experiments and Simulation of Devices” (2014). He has received multiple awards among which it is highlighted that, in 2016, he was awarded the Zeno Karl Schindler prize in the Field of Environmental Sciences and Sustainability thanks to his postdoctoral work. Wolfgang was a Marie-Curie fellow at the Ludwig Maximilian University in Munich and a Ambizione Fellow at the École polytechnique fédérale de Lausanne. He is also a member of the editorial board of the open access journal “Research in Advanced Energy and Sustainability”. His research is focused on the physics of perovskite solar cell devices; and more recently he has investigated phenomena of recombination and hysteresis in this system.

Abstract:

In the last decade, metal-halide perovskite semiconductors have received tremendous attention in research due to their excellent optoelectronic properties, making them highly interesting materials for solar cells and light emitting diodes (LEDs). It is fascinating that these perovskites are highly tolerant against electronic defects, which allowed for solar-cell efficiencies greater than 25% and at the same time show ionic conductivity mediated through mobile lattice defects.

In this talk the device physics of perovskite solar cells is discussed. Focus is on the peculiar properties of the material, which enable low recombination losses and thus high photovoltages. Furthermore, the various effects of ion migration on device performance are described. They range from hysteresis in the current-voltage curve of solar cells, to reversible degradation during long-term operation, to high gains in photodetectors and the electroluminescence in LEDs that depends on the mode of operation.

Key in understanding these phenomena is the interplay between ionic and electronic conductivity, where the ionic response belatedly modifies the electronic response, which is the one commonly observed in devices.

This interplay has consequences on how to interpret the results of common characterization techniques. In addition, the real-world long-term operation of perovskite optoelectronic devices under varied ambient conditions is affected. These points lead towards the open challenges, which conclude the talk.

A BRIEF LOOK INTO ELECTRON MICROSCOPY: UNVEILING MATERIALS PROPERTIES AT THE ATOMIC AND NANOMETER LEVEL

DR. JUAN CARLOS IDROBO

Biography:

Juan Carlos Idrobo is a Senior Staff Scientist at Oak Ridge National Laboratory and Group Leader of the Scanning Transmission Electron Microscopy Group at the Center for Nanophase Materials Sciences. His research consists in applying analytical techniques in electron spectroscopy within monochromated and aberration-corrected scanning transmission electron microscopy to study the structure and electronic, magnetic, thermal, optical and topological properties of materials. He has published over 170 papers in peer review journals with over 16,000 citations. In 2018 Idrobo was recognized by Clarivate Analytics to be among the top 1% of researchers being cited in Cross-Field in Web of Science, between 2006 and 2016. Idrobo holds Physics degrees from Universidad de Los Andes in Colombia (B.Sc., 2000), University of Illinois at Chicago (Master, 2003) and University of California Davis (Ph.D., 2004).

Abstract:

Modern scanning and transmission electron microscopes (S/TEM) are now almost ubiquitous in materials and biological sciences laboratories. They have radically enhanced our understanding of organic and inorganic matter with the successful development of aberration correctors [1,2], detectors with film-equivalent dynamical range [3], and more recently, with monochromators capable of achieving sub-10 meV energy resolution spectroscopy [4].

Here, I will present several examples demonstrating how we have exploited these capabilities and solved the pertinent experimental challenges to probe materials behavior at the nanometer and atomic scales. Specifically, I will show how by utilizing the phase of the electron probe one can reveal the magnetic order of complex-oxide materials at the atomic level. I will also explain how the new generation of monochromators, combined with aberration-corrected STEM, can be used (i) as a primary thermometer (without requiring any previous knowledge of the sample) [5].

I will also explain how the new generation of monochromators, combined with aberration-corrected STEM, can be used (i) as a primary thermometer (without requiring any previous knowledge of the sample) [6]; and to detect site-specific isotopic labels in amino acids at the nanometer scale [7]. Additionally, I will show how one can now visualize the electric field of individual atomic columns of heavy and light elements, detect charge density inhomogeneities and the magnetic order of materials at the sub-Angstrom scale by using an ultra-low noise SCMOS detector in the diffraction plane [8].

Lastly, I will discuss potentially relevant new challenges in electron microscopy. For instance, will it be possible to map orbitals and spins with atomic resolution and with single atom sensitivity; detect a superconducting transition; measure the

specific heat and thermal conductivity of materials; map Hall effects or topological properties with nanometer resolution [9]? These questions will be addressed and further elaborated during the presentation [10].

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CULTURAL ACTIVITIES

A VIRTUAL TOUR OF THE GALAPAGOS ISLANDS

MSC. DANIELA COX

Biography:

Daniela Cox is a third generation from Galapagos linked to cultural and environmental initiatives of her island community from an early age. Master in Sustainable Business from Griffith University, Community Organizer in Wilderness Society Australia, Naturalist Guide of the Galapagos National Park, Municipal Environmental Director, youngest woman elected politician in Galapagos. Since 2019 he has lived in Denmark with his family, he is a member of the Nordic B Leaders Network, promoter of Regeneration, Ex Advisory Board of Women 4 Solutions, and CEO of Plura Consulting, the Galapagos-Scandinavian firm that helps individuals and organizations to integrate and experiment sustainability and regeneration from a holistic and systemic vision. Due to her multisectoral trajectory and her activism in Sustainability and Diversity, Daniela is a local and international speaker and presenter

Abstract:

Almost a thousand kilometers away from South America, Galapagos is a dynamic, unique and fascinating archipelago of the Ecuadorian territory. The natural wealth of its geography, geology and ecology harmonizes with the consciousness, resilience, and adaptability of its island population. What are the challenges and opportunities for regenerative and mindful post-pandemic tourism? What ecosystems does the marine reserve sustain for conservation and for economies in the region? And how its island history and culture are the key to building new community narratives anywhere. Join Daniela Cox in a photographic presentation with a local and global perspective on Galapagos, in an invitation to learn more about the Enchanted Islands, which inspired Charles Darwin.

ORAL CONTRIBUTIONS

Astronomy

Astronomy for development: Astrostays in the middle of the world

Oral
contribution

Nicolás Vásquez¹, Marcela J. Morillo Acosta², Andrés Baquero, Raúl Puebla

¹Escuela Politécnica Nacional;²Universidad Técnica de Cotopaxi

Abstract

“Astronomy for Development is about PEOPLE, not the STARS” The Andean Regional Office of Astronomy for Development of the International Astronomical Union motivates local astronomers to use technical skills to solve social problems. The pandemic restricted people’s mobility, however an increase in tourism is expected to recover all over the world. Ecuador, recognized as an attractive travel destination, has more natural sites to visit than the Galapagos Islands, nevertheless, continental and rural regions remain still unexplored. La Chorrera, located near the Equator, is a poor fisherman village with welcoming customs. Although it is known for its gastronomy and beautiful beaches, it lacks places to stay making the experiential tourism underdeveloped. Tourists look for an immersion travel but the host conditions are under-qualified. Being in the neighborhood of the equatorial line, it is a perfect place to observe the sky and learn about the astronomical history of Ecuador. The first geodesic mission landed in this coastal in 1736, and the environment remains preserved to nowadays. Current project aims to develop (1) experiential tourism in La Chorrera, and (2) to create a space for undergraduate students to acquire social ability and use technical skills learned in their institutions for the benefit of the community. This project will restore and adapt local houses to receive tourists to stay overnight and additionally offer an experience based on astronomical features and fishermen culture. For this purpose, members of Ecuadorian universities will develop guides, digital platforms, and provide training to community members on topics regarding astronomy and everyday physical phenomena. This initiative aims to complement the ongoing project of the Coaque Astronomical & Archaeological Museum and contribute in the sustainable rural tourism. The developmental goal focuses on the idea of building sustainable and decent work possibilities for the inhabitants of La Chorrera and nearby coastal equatorial region, involving academics in the solutions of social problems of Ecuador.

Reference

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ZTF constraints on variability from intermediate-mass black hole candidates

Oral
contribution

Ernesto Camacho¹, Paula Sánchez-Sáez, Franz Bauer, Paula Sánchez-Sáez

¹Pontifical Catholic University of Chile

Abstract

Probing massive black holes into the intermediate-mass black holes (IMBH; $\sim 10^4 - 10^6 M_{\odot}$) regime has seen significant progress in the last two decades. It is thought that IMBHs could give insight on the origin and evolution of modern-day supermassive black holes. Moreover, they are the perfect candidates to test the relations between black holes and their host galaxy. With LSST's enormous potential, in terms of data quality and quantity, we expect that the sample of IMBHs candidates may increase by at least 2 orders of magnitude with long, well-sampled, light curves. In order to understand the processes involving IMBHs, and prepare for LSST-like data, we analyzed Zwicky Transient Facility (ZTF) forced photometry of three IMBHs samples e.g. Greene & Ho (2007b), Dong et al. (2012), Chilingarian et al. (2018). The joint sample comprises ~ 534 candidates with broad-line masses $3 \times 10^4 < M_{BH} < 2 \times 10^6 M_{\odot}$. It is expected that as the black hole mass decreases, more rapid variability will be observed. After cleaning each forced photometry light curve and performing various quality control checks, we characterize the variability signatures using a variety of estimators and relate them to the physical properties of the sample. While some candidates show strong and fast variability as expected, others do not. We will present our results and discuss possible scenarios, particularly as they relate to prospects for LSST.

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Characterising cosmic filaments using hydro-dynamical simulations

Oral
contribution

Daniela Galárraga-Espinosa¹

¹Institut d'Astrophysique Spatiale

Abstract

Matter in the Universe is assembled under the action of gravity to form a gigantic network of nodes, filaments, walls, and voids, called the cosmic web. This structure is mainly set by the dynamics of dark matter (DM), which forms the skeleton onto which baryonic (or ordinary) matter is accreted. While the denser cosmic structures (clusters of galaxies) have been thoroughly studied, because of their lower densities and complex morphologies, cosmic filaments and the properties of matter around them are still poorly known. However, these structures are believed to contain almost half of the matter in the Universe. The study of matter at the largest scales is therefore inevitably linked to that of filaments. I will present a comprehensive study of cosmic filaments today, detected in recent large-scale hydro-dynamical simulations. The radial distribution of DM, gas, and galaxies is analysed, together with the temperature and pressure of gas around these structures. I will show that filaments of different lengths do not have the same properties, leading to the identification of two extreme populations: short ($L_i < 9$ Mpc) and long filaments ($L_i > 20$ Mpc). I find that short filaments are denser, puffier, and hotter than the long ones. The two populations thus trace different environments in the cosmic web: while short filaments correspond to the bridges of matter between over-dense structures, the long ones are at the basis of the cosmic skeleton, often embedded in under-dense regions. Despite the differences between populations, I will also show that all filaments are essentially made of gas in the warm-hot intergalactic medium (WHIM), their cores are isothermal with a temperature of $T_{core} = 4 - 13 \times 10^5 K$, and their pressure is ~ 1000 times lower than in clusters of galaxies. Finally, I will present an estimation of the Sunyaev-Zel'dovich signal of filaments that is compared with recent observations from Planck data.

Reference

Populations of filaments from the distribution of galaxies in numerical simulations, D. Galárraga-Espinosa, N. Aghanim, M. Langer, C. Gouin and N. Malavasi, 2020, A&A, 641, A173

Properties of gas phases around cosmic filaments at $z = 0$ in the IllustrisTNG simulation D. Galárraga-Espinosa, N. Aghanim, M. Langer and H. Tanimura, 2021, A&A, 649, A117

Relative distribution of DM, gas and stars around cosmic filaments in the IllustrisTNG simulation D. Galárraga-Espinosa, M. Langer and N. Aghanim, 2021, submitted to A&A

Extragalactic Fast X-ray Transient Candidates Discovered by Chandra

Jonathan Quirola¹, Franz Bauer

¹Pontificia Universidad Católica de Chile

Abstract

Fast X-ray Transients (FXRTs) are as-yet unexplained phenomena. They are energetic X-ray flares that last a few tens to a few thousand seconds. Over the past few years, ~ 30 extragalactic FXRTs have been discovered in Chandra, XMM-Newton, Swift/XRT, and eROSITA data. Numerous proposed explanations include a tidal disruption (TDE) of a white dwarf (WD) by an intermediate-mass black hole (IMBH), a supernova shock breakout (SBO), and a binary neutron star merger (BNS). So far, FXRTs lack multiwavelength counterparts, and hence we rely on their host properties to understand their nature. In this talk, I will present a new population of FXRTs serendipitously discovered from Chandra archival data (observation from the Chandra Data Release 2 and beyond 2015). This new sample of 14 FXRTs might have a mix of origins. We identify a sub-sample of FXRTs that show similar timing and spectral properties to CDF-S XT2 (a FXRT previously identified in the Chandra Deep Field South), and volumetric rate density, which suggest an association with BNSs. The improve in the detection of FXRTs by the current and future X-ray missions will open new opportunities to study and understand exotic astrophysics phenomena associated with FXRTs.

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An overview of shock-multicloud interactions in magnetised galactic winds

Oral
contribution

Wladimir Eduardo Banda-Barragán¹

¹Universität Hamburg

Abstract

Galactic winds are multi-phase outflows that remove gas from star-forming galaxies. Observational studies of such winds have found evidence of fast-moving, cold, dense gas located at large distances from the host galaxies. However, the origin of this cold phase is still debated between advection and in-situ formation scenarios. Here, I discuss how condensation occurring within a dynamical, turbulent wind can intrinsically sustain a long-lived cold phase. I describe the thermodynamical evolution of dense gas clouds embedded in magnetised galactic winds. Using 3D magnetohydrodynamical simulations of radiative multicloud layers interacting with strong shocks, I show that: a) radiative clouds become efficiently mixed and develop filamentary morphologies, b) entrained gas retains some information of the initial density distribution of the multicloud layers, c) strong radiative cooling replenishes dense gas along the wind, and d) magnetic fields offer little extra stability in weak-field models, but they can alter the morphology of the post-shock flow depending on their strength and topology. Therefore, I show that the interplay between radiative heating and cooling ensures that warm and cold gas clouds coexist with hot gas in a multi-phase flow. At the end, I compare the dynamical and morphological properties of outflowing gas in my simulations to those of the atomic gas phases in observed galactic winds.

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Equatorial total electron content

Ericson López¹, Erik Toapanta, Hugo Barbier¹

¹Escuela Politécnica Nacional de Ecuador

Abstract

The total electron content (TEC) is a parameter that quantifies the Earth's ionosphere state, which influences the propagation of electromagnetic waves which pass through. Measuring the total electron content of the ionosphere is relevant in the investigation of ionospheric morphology since innumerable physical processes take place in the upper atmosphere. One of the tools used to measure TEC is the global positioning system (GPS). GPS is a satellite-based radio navigation system that is used to verify the position in real-time with an error of a few centimeters. A relevant aspect of TEC's study is that allows a better understanding of the spatial and temporal variation of the ionosphere, thus allowing the implementation of new tools to make more precise ionospheric corrections in satellite communication and navigation systems. This article presents the methodology used for the calculation of the total electron content of the equatorial ionosphere for a period from 1999 to 2019, using the carrier phase and pseudo-range parameters, which were obtained from a NASA archive. An additional contribution of this work is the estimation of the equatorial geomagnetic field from a slight modification of the standard theoretical TEC model.

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Evaluation of the survival probability of exoplanets orbiting low-mass stars with enhanced energy loss

Oral
contribution

Santiago Arceo Díaz¹, Elena Elsa Bricio Barrios, Kai Zuber

¹Tecnológico Nacional de México

Abstract

We analyze the survival probability of exoplanets orbiting low-mass stars through their evolution from main-sequence to towards the white dwarf phase. We focus on the effect that the possible production of neutrinos, with a magnetic dipole moment and milicharge, and axions could have on the final stellar radius, luminosity, and mass-loss rate and how this could, in turn, affect the orbital evolution of planets orbiting low-mass stars. The numerical stellar models, created with the Eggleton stellar evolution code, and an n-body algorithm, in which tidal drag and dynamical friction are considered, are used to calculate the minimum safe distance for different configurations and number of exoplanets. . Two exoplanet systems, known for harboring single red giant stars, were modeled by using the predicted stellar properties to calculate the temporal variation of the habitable zone and the orbital distance.

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Complex systems

Oral
contribution

Primary cycles in complex networks

Ramon Xulvi-Brunet¹

¹Escuela Politécnica Nacional

Abstract

Complex networks is a young area of research that, inspired by empirical findings of real-world systems such as the so-called social networks, the brain, sets of interconnected computers, biological relationships among proteins, etc, tries to characterize and model the evolution of systems of many interacting elements, as well as to understand dynamical processes that take place on these many-parts systems, such as, for instance, epidemics and synchronization. When talking about network characterization, most biological, technological, and social networks display substantial non-trivial structural features that, to a certain degree, reflect the interacting properties of the different elements of which those systems are made of and that the networks represent. Such structural (or most precisely, topological) features include, just to mention a few of them, the so-called degree distribution, the clustering coefficient, the degree-degree correlations, and the community and hierarchical structures. Despite the advances made in the past two decades in characterizing the structure of networks by means of the above-mentioned topological measures (and others that have also been introduced and successfully used, but that we do not have mentioned), a set of measures capable of completely characterizing any possible network topology is still missing. Independently of whether this ambitious goal will ever be achieved or not, the introduction of new and suitable topological measures aimed at better characterizing the structure of networks is always a task that we must try and look for as researchers of the area. In this talk, I would like to introduce the concept of primary cycles and provide an algorithm capable of counting all of them as a function of their length, i.e. an algorithm capable of determining the distribution of these primary cycles. By means of this algorithm, I will show, after applying it to a few networks, how this primary cycle distribution can help characterize some aspects of the topology of networks.

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Statistical Analysis Of Pseudo-Local Properties In Turbulent Space Plasmas Using 3d Numerical Simulations

Oral
contribution

Rocio Elizabeth Manobanda Guamán¹, Luca Sorriso-Valvo², Renaud Ferrand,
Christian Leonardo Vásconez Vega

¹Universidad Técnica de Ambato;²National Research Council

Abstract

The Solar Wind (SW) is a turbulent plasma emitted by the Sun that is permeated in interplanetary space and it is in constant interaction with our planet's magnetic field. This medium is characterized by its low inter-particles collisions rate, and it has been extensively studied in the last decades. However, the physics of the dissipative mechanisms present at these small scales, and the different dissipation processes triggered by them, are still a matter of research [2]. It stands as a colossal natural laboratory that boasts extremely rich physics, most of it still remaining to be fully understood. The sole study of the turbulent phenomena at work at the multiple scales of the SW represents a full-edged challenge, and a great opportunity to hone our understanding of plasma turbulence in general. Since the second half of the last century, space missions have recorded a large number of in situ measurements, directly within the SW or its incursions in terrestrial magnetosphere, providing a detailed description of the state and dynamics of the plasma. In order to understand the characteristics of the active dissipative mechanisms in this medium, precise knowledge of the fluctuations that make energy available for small-scale conversion is required, since different dissipation processes are triggered by fluctuations of different nature [2]. Consequently, a wide range of theoretical and computational methods have been developed to analyze the resulting data. In recent years, direct numerical simulations, where novel statistical analysis and models can easily be tested, have been a valuable support to satellites and spacecraft observations. In-situ measurements of space plasma have shown a turbulent cascade transporting the energy injected at the magnetohydrodynamic (MHD) scales towards the dissipative scales [1,2], through the inertial range. In [4] it has been shown that the observed fluctuations in magnetohydrodynamic plasma turbulence follow the Politano-Pouquet law. In this work, we present the first pseudo-local analysis, using the Local Energy Transfer (LET) proxy [3], in a three-dimensional direct numerical simulation of a quasi-turbulent plasma. The scale-by-scale properties of the different "energy" channels are estimated using the LET parameter, which is based on the third order moment scale law for Hall-MHD. The isolated structures found in this study could be interpreted as manifestations of intermittence localized at turbulent dissipation locations. Finally, a comparison with recent results, from a 2D turbulent case-of-study, presented in [4] is discussed.

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Oral
contribution

Newton-Prigogine y la inter-ciencia

David Guzmán¹
¹PUCE

Abstract

In this work we propose to address the inter-scientific dialogue. The reflection that Ylia Prigogine raises about the place of physics –that is, of Newton- in relation to the other sciences and to philosophy implies a reorganization of academic knowledge. If during the 19th and 20th centuries physics was adopted as a model for the other sciences, what Prigogine does is re-establish the dialogue between the sciences and the dialogue between the sciences and philosophy, and by extension the humanities.

Reference

Prigogine, Ylia, *La nueva Alianza*, Madrid, Alianza editorial: 1971

Oral
contribution

Statistical properties of Ecuadorian seismicity

Ramon Xulvi-Brunet¹, Stephen Hernández, Luca Sorriso-Valvo, Mario Calixto
Romero Ruiz¹

¹Escuela Politécnica Nacional

Abstract

Ecuador is located next to and straddles an active plate tectonic boundary that makes the country prone to earthquakes of significant magnitude. As urban areas continue to sprawl and a larger percentage of the country's population begins to occupy areas of high seismic hazard, it is increasingly important to characterize the seismic risk these areas are subject to. As part of the internal project PII-DFIS-2019-07, this study takes a multi-pronged approach to analyze Ecuadorian seismicity.

We base our analysis on a catalog of 25k earthquakes of magnitude ≥ 2.8 and spanning the period between 2013 and 2021. Using this catalog, we conduct a series of spatial and temporal analysis to better understand and contextualize the statistical properties of our dataset. For our spatial analysis, we subdivide our catalog into 10 distinct non-overlapping seismo-tectonic provinces, chosen such that their source properties and underlying dynamics are generally distinct from one another. For the time series, we conduct 3 distinct analyses: statistical assessments of the Gutenberg-Richter (GR) and Omori Laws, and a multifractal assessment of the catalog. For all three statistical analyses, we assess the catalog as a single whole, the catalog with shallow and deep seismicity as distinct wholes, and the catalog separated into 5 shallow and 5 deep seismo-tectonic provinces. Finally, we develop a novel computational model to reproduce the underlying earthquake mechanics. With respect to the Gutenberg-Richter relation, deep seismicity tends to have a lower exponent and is thus indicative of a higher stress environment at depth. For the Omori Law, because of mixing of different tectonic provinces, the classical power law indicative of an Omori relation is broken and cannot be reproduced. This is not unexpected since no attempt is taken to decluster the catalog hence there is no obvious way to distinguish between background seismicity and aftershocks. For our multifractal analysis, we find that in general the shallow events have a larger multifractal parameter (0.69) than the intermediate depth events (0.50). This indicates a large heterogeneity in the shallow seismicity relative to deep. When subdivided into 5 shallow provinces, and 5 deep provinces, only 4 shallow and 1 deep province contain enough data to confidently characterize its fractal dimension, with the shallow provinces generally showing higher fractal dimension on an individual basis. This indicates a need to include more data and/or characterize more carefully the seismo-tectonic provinces in this study. Finally, we obtain initial computational model results that reproduce in a broad sense a Gutenberg-Richter magnitude distribution. For future work, we hope to tune this computational model so that it lies in closer agreement with the statistical analyses of the real Ecuadorian catalog summarized above.

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3D on-lattice stochastic reaction-diffusion simulation of protein-membrane reversible association

Lupe Villegas¹, Jose Requejo-Isidro

¹Centro Nacional de Biotecnología (CNB), CSIC.

Abstract

Protein-membrane interactions are fundamental in many biological issues. Determining the magnitudes of those interactions and understanding the processes have a high importance in biology. In particular, we were interested in the dynamics of adhesion of antibodies to Human Immunodeficiency viruses (HIV), but our proposed method is more general. Current computational methods to describe those process microscopically require a high cost and time. We present an alternative mesoscopic method using the Reaction-Diffusion Master Equation (RDME) to model interactions between proteins and the viral membrane. RDME gives a general approximation of the behavior of a system and can be studied by numerical algorithms. We consider two types of interactions: diffusion and reaction. The molecules follow random trajectories, i.e., they diffuse. In addition to that, following certain reaction rules given a priori, the molecules react when they encounter in space. We have solved numerically the proposed Reaction-Diffusion Master Equation by using the Next Subvolume Method, instead of simulating all the trajectories of all the molecules of our system, we will place the molecules in “sub-volumes”. The molecules will diffuse from one sub-volume to another, and molecules in the same sub-volume will be able to react with each other. The method has been applied to a system composed by spherical molecules (0.5 nm of radius) called “antibodies” that can be stucked to bigger spherical molecules (50 nm of radius) called “virions”, both types of molecules are moving with specific diffusion constants in a micrometric box. Additionally, we use mean-field theory to solve the non-linear equations for the macroscopic evolution of the system. These solutions of the equations gave us information about the equilibrium concentration. We have observed a meta-stable state characterized by a Poisson distribution and a final equilibrium state given by an exponential distribution. The meta-stable state was analyzed from solving differential equations using mean-field theory.

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Condensed matter physics

Influence of dopamine on the magnetic properties of superparamagnetic iron oxide nanoparticles

Oral
contribution

Jilder Dandy Peña Serna¹, Miguel Novak, Claudio Sangregorio, Benjamin Rache Salles, Martin Albino, Oana Pascu, Davide Peddis, Oana Pascu

¹Centro Brasileiro de Pesquisas Físicas

Abstract

We report on the effect of different molecular coating as carboxylate and catecholate ligands on the magnetic properties of small (average 4.4 nm) iron oxide nanoparticles (NPs) prepared by the thermal decomposition method using oleic acid as stabilizer followed by dopamine ligand exchange step [1]. We investigated the role of the surface chemistry of ligand stabilized NPs and their overall resulting magnetic properties. To isolate the contribution of the NPs from the coating, the ligand percentage in contact with iron oxide surface is evaluated by thermogravimetric measurements. Our M(H) measurements at room temperature show a superparamagnetic behavior for all samples and ZFC-FC magnetization curves and AC magnetic susceptibility measurements indicate a decrease of magnetic interaction after ligand exchange. The insight about the surface effect on NPs magnetic properties is obtained through X-ray absorption spectroscopy (XAS) and X-ray circular magnetic dichroism (XMCD) measurement [2]. The modification of the Fe L_{2,3} XAS and XMCD line shape upon ligand substitution extent show the change of Fe cations distribution between octahedral and tetrahedral sites with the ligand exchange.

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Electric multipole moments in crystalline insulators

Rodrigo Sandoval¹, Leonardo Basile¹, Wladimir Benalcazar

¹Escuela Politécnica Nacional

Abstract

The macroscopic polarization is the most essential concept in any phenomenological description of dielectric materials, but calculating this and other electric multipole moments in crystalline insulators is not an obvious process due to the quantum mechanical behavior of the electron cloud and the periodicity of the lattice. In this project, we will study how the first three electric multipole moments are related to each other in crystalline insulators. For this purpose, we will use the tight-binding SSH (Su-Schrieffer-Heeger) model, that represents a one-dimensional crystalline insulator, and the tight-binding QTI (Quadrupole Topological Insulator) model, that represents a two-dimensional crystalline insulator. We will verify that the one-dimensional model presents a quantized electric dipole moment that generates charge accumulations at the ends of the crystal, while the two-dimensional model presents a quantized electric quadrupole moment that generates charge accumulations at the corners of the crystal, as well as polarizations at its edges. In order to compute the electric dipole moment, we will use the quantum mechanical operator of the position in one dimension, as well as an analogous operator in two dimensions to calculate the electric quadrupole moment. Finally, to check the generality of the operators used in our algorithm, we will verify that the first three multipole moments in the QTI model behave as predicted by the theory, even when the quadrupole moment is not quantized. Due to the fact that both models are topological insulators, they have promising applications to produce more efficient electronics and to construct stable quantum computers.

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Structural and Thermal Properties of InSb:Mn with MnSb Clusters

Oral
contribution

Jesús González-Laprea¹, Eduardo Quintana, Jaime A. Castro, José R. Fermin²,
Carlos Durante², Martín Emilio Mendoza Oliveros

¹Pontificia Universidad Católica del Ecuador;²University of Zulia

Abstract

III-V family compounds doped with transition metals are promising materials for spintronic applications. Synthesis of an In_{0.9}Mn_{0.1}Sb ingot was thus carried out by direct fusion of the stoichiometric mixture of the constituent elements, followed by controlled cooling. The ingot obtained showed p-type conductivity. Scanning Electron Microscopy (SEM) images show MnSb clusters in an InSb matrix doped with Mn, a result like that found when the compound is obtained using other techniques. Energy-dispersive X-ray spectroscopy (EDS) shows that the atomic ratio of the clusters is Mn/Sb = 0.896 +/- 0.025, while the atomic ratio of the matrix is In/Sb = 1.013 +/- 0.005. The indexation of the powder X-ray diffraction pattern at room temperature yielded a majority cubic phase of InSb doped with Mn, with a lattice parameter $a = 6.474173 \text{ \AA}$ and cell unit volume $V = 271.36 \text{ \AA}^3$, while non-indexed reflections are associated with the presence of MnSb rich in Sb. The phase transition temperatures were obtained from differential thermal analysis (DTA) measurements on powder samples in evacuated quartz ampoules. It can be observed that fusion of the InSb matrix doped with Mn occurs between 485 °C and 528 °C, unlike the congruent fusion of the InSb at 527.7 °C; while the fusion of the Sb-rich MnSb clusters occurs between 494 °C and 509 °C. These temperatures are lower than those reported for the Sb-rich side of the phase diagram of the Mn-Sb binary system, which shows a decrease in the compounds' thermal stability. The estimated fusion enthalpies for InSb:Mn and antimony-rich MnSb are, respectively, 4.8 Kcal/mol and 117.4 Kcal/mol.

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Improving the electrical properties of graphene inks by controlling nanosheet thickness distribution

Jimmy Narváez¹

¹Escuela Politécnica Nacional

Oral
contribution

Abstract

Electrochemical exfoliation has become an essential tool to obtain graphene inks for different electrical and electronic applications. In this contribution, the resistivity of spray-coated graphene films constructed from inks are evaluated. In particular, a

comparison of electrical properties of two types of graphene films are presented: i) films incorporating graphene nanosheets with a wide thickness distribution (5 ± 4 graphene monolayers) as prepared from electrochemical exfoliation of bulk graphite and ii) films incorporating graphene nanosheets obtained by application of the liquid phase cascade centrifugation (LCC) to nanosheets prepared by electrochemical exfoliation; where, a narrower thickness distribution (6 ± 2 graphene monolayers) is achieved. The characterization of these films reveals that electrical resistance depends on the nanosheet thickness distribution. A broad thickness distribution conducts to high resistance values, $10.30 \text{ k}\omega/\text{m}^2$; whilst, a narrower thickness distribution leads to a lower resistance, $5.81 \text{ k}\omega/\text{m}^2$. These results demonstrate that the LCC technique can be used to classify graphene nanosheets controlling the electrical properties of the graphene inks. This methodology paves the way to scale the production of graphene through a simple and low cost procedure. This graphene could be used in several applications where electrical conductivity of the graphene nanosheets plays a fundamental role.

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Molecular dynamics algorithm for simulating KeV particles bombardment

Ramon Xulvi-Brunet¹

¹Escuela Politécnica Nacional

Abstract

Classical algorithms for molecular dynamics are nowadays important in studying many different branches of physics and other sciences, from studying the dynamics of biomolecules to analyzing surfaces and manufacturing semiconductors. Most applications of molecular dynamics algorithms are on systems composed of N particles that interact with each other by means of a set of forces that do not significantly change their strength during the whole simulation time (or, at least, no excessively strongly). These common algorithms are mostly used in “liquid” simulations with fixed integration time steps, since fixed integration time steps appear to be adequate for simulating such type of systems. On the other hand, for simulating the bombardment of solids by energetic, charged particles, where the bombarding particles are usually submitted to extremely high potentials within very short periods of time (compared to much more weak potentials during the most part of the simulation), it is known that a fixed integration time step is quite inefficient, if the integration step is sufficiently small, or inadequate, if the integration step is not sufficiently small. An example of this situation is the bombardment of solids by energetic electrons (possibly, with an energy of the order of KeV), where the electrons are submitted to very strong forces only when they are close enough to other particles of the solid. For simulating such types of systems thus becomes essential to design molecular dynamics algorithms with adaptive integration time steps. We present a variable time step integration algorithm capable of simulating the “hard collisions” of energetic particles, i. e. the dynamics of energetic particles submitted to high potentials for very short periods of time. This adaptive algorithm is a fourth order algorithm that needs to evaluate the interaction forces only once per time step. The algorithm is tested on some model problems that have exact solutions and compared against the common velocity Verlet method.

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Electrical characterization of molecular junctions using graphene obtained by electrochemical exfoliation

Oral
contribution

Esteban Humberto Yépez Jiménez¹, Henry Marcelo Osorio Calvopiña¹

¹National Polytechnic School

Abstract

Molecular electronics is a potential candidate to replace current silicon-based technology; and thus, continue the ongoing trend toward miniaturization of electronic devices. This technology is based on the formation of electronic devices from a molecule connected between two or three electrodes. Among other challenges, research in this field has focused on applying several techniques for making and characterizing metal-molecule-metal junctions. These have been used to understand the charge transport in the metal-molecule-metal junction. Generally, gold has been used as electrodes for electrical characterization of these molecular junctions; however, the growing concern for the environment has forced our attention on the use of novel, cheaper and biocompatible materials. In this context, electrochemically exfoliated graphene appears as an important alternative for use in several electronic applications, including molecular electronics. In this work, graphene nanosheets have been obtained by electrochemical exfoliation and subsequent liquid phase cascade centrifugation technique. These nanosheets have been used for the construction and characterization of metal-molecule-graphene junctions using the scanning tunneling microscopy break junction (STM-BJ) method. Results are compared with those obtained in typical metal-molecule-metal junctions. Our experimental results show that electrical conductance at the molecular junction is similar when using graphene compared to gold as electrodes.

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Parametric X-ray Radiation from nano meter powders

Esteban Irribarra¹, A.S. Kubankin, A. N.Eliseyev, R.M. Nazhmudinov, A.S. Kluev, V. I. Alexeyev, R.M. Nazhmudinov, Kishin Ivan², A.S. Kluev

¹Escuela Politécnica Nacional;²Belgorod National Research University

Abstract

Parametric X-ray Radiation PXR is generated when charged particles interact with periodic structures. The Coulomb field of the incident charged particles excites the bounded electrons which emit radiation that coherently interferes in some directions and for certain energies. The characteristics of the radiation depend on the incident charges particles, the observation angle but also on the characteristics of the sample being used [1]. For this reason, the radiation generated in crystals differs substantially from that observed in polycrystals and finally, PXR is not generated in amorphous media since destructive interference is observed in all directions [2-5]. In this talk, we present the experimental results of the interaction of a 7 MeV electron beam with platinum powder constituted from grains which main dimensions were around 5.2 nm +- 1.4 nm. The experimental results were compared with theoretical predictions for PXR produced in randomly oriented crystallites [4]. It is important to mention that theory considers that the size of the crystallites is large enough, and the sample is half infinite to guarantee that the radiation is generated at saturation. A good agreement between the experimental results and the theoretical predictions is observed even when in our case, the crystallite dimensions are smaller than the attenuation length of X-ray in the sample for a given energy.

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ZnO thin films grown at low temperature by PE-ALD for application in electronic devices

Oral
contribution

Jhonathan Rafael Castillo Saenz¹, Marcelo Martínez Puente, Eduardo Martínez Guerra, Mario Alberto Curiel Álvarez, Francisco Servando Aguirre Tostado, Eduardo Martínez Guerra, Nicola Nedev, David Mateos, Benjamín Valdez-Salas, Oscar Perez-Landeros, María Isabel Mendivil Palma²

¹Universidad Autónoma de Baja California;²Centro de investigación en materiales avanzados S. C.

Abstract

ZnO layers with thicknesses of 20, 40 and 60 nm were deposited by Plasma Enhanced Atomic Layer Deposition (PE-ALD) at 70 °C. Diethylzinc (DEZ) was used as organometallic precursor, O₂ and H₂O as oxidant agents and Ar as a purge gas. The deposition cycle consisted of 100 ms DEZ pulse, 10 s purge time, 6 s of plasma oxidation at 200 W and 10 s purge time. The optical constants and thicknesses of the grown layers were determined by spectroscopic ellipsometry, while the roughness was measured by atomic force microscopy, giving average roughness values in the 0.20 – 0.22 nm range for films deposited under different conditions and having different thicknesses. The optical band gap of the films are 3.22 and 3.23 eV for H₂O and O₂ plasma, respectively. A high optical transmission (90 %) was measured by UV-Vis spectroscopy. X-ray diffraction exhibit the formation of polycrystalline patterns with (100) and (002) predominant planes. X-ray photoelectron spectroscopy revealed a high purity of the obtained ZnO films, no carbon was detected. The obtained excellent optical, morphological and compositional properties of the deposited films, make them a promising candidate for electronic and optoelectronic applications, which require low temperature processes.

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Adsorption enhanced photocatalytic degradation of Rhodamine B using $Gd_xBi_{1-x}FeO_3@SBA-15$ ($x = 0, 0.05, 0.10, 0.15$) nanocomposites under visible light irradiation

Maria Jose Benitez¹, Sofia Andrade, Karla Sofia Vizuite Armendáriz², Valeria Ochoa, Thomas Cadenbach³, Alexis Debut²

¹Escuela Politécnica Nacional;²Universidad de las Fuerzas Armadas ESPE;³USFQ

Abstract

BiFeO₃ nanomaterials have recently generated much interest due to their relatively narrow band gap energies (2.0–2.8 eV), their stability and low cost which leads to effective visible-light photocatalysts for water splitting and for the degradation of organic pollutants. Here, we show that very high removal efficiency of the organic dye Rhodamine B can be achieved using $Gd_xBi_{1-x}FeO_3@SBA-15$ nanocomposites ($x = 0, 0.05, 0.10, 0.15$) under visible light irradiation. Specifically, we study the photocatalytic degradation of Rhodamine B using the above nanocomposite materials, with pore volume loadings of 5–25%, prepared by a wet-impregnation nanocasting technique with pre-fabricated metal tartarates, as metal precursors, and mesoporous silica SBA-15, as a host matrix. We find that the best removal performance is achieved by a 10 vol% $Gd_{0.05}Bi_{0.95}FeO_3@SBA-15$ sample, shown by a complete dye degradation in approximately 3 h using very low concentrations of the actual active photocatalyst. The superior efficiencies of the nanocomposites, which outperformed their parent compounds, i.e. $Gd_xBi_{1-x}FeO_3$ nanoparticles as well as unfilled SBA-15, are attributable to a synergistic adsorption enhanced photocatalytic degradation process.

Reference

T. Cadenbach et al., *Ceramics International*, 47, 29139 (2021)

Catalyst dependency on the growth of single-walled carbon nanotubes

Carlos Reinoso¹, Luis Corredor¹, Roberto Andrade

¹University YachayTech

Abstract

The carbon nanotubes synthesis has been largely studied in the last decades, especially due the importance of its optical, electrical and mechanical properties that let us envisage promising applications in science and engineering. The improvement in finding the optimal conditions for its fabrication are still in development, this comes together with the necessity of the well understanding of its growth at atomic and molecular level. Among the more interesting properties are the response as metallic or semiconductor behavior of single-walled carbon nanotubes that are

related just within its geometry [1]. In this work we report, to the best of our knowledge, the first synthesis of SWCNTs made in Ecuador by chemical vapor deposition CVD. Characterization was carried out using mainly Raman spectroscopy due the facile inspection related with the molecular vibrational modes of the sp² carbon hybridization [2]. X-ray diffraction XRD and X-ray photoelectron spectroscopy XPS were used to catalog the catalyst under study giving a deep insight of its chemical composition and environment before and after activation that allow us to correlate it with its Raman Spectra [3]. The best temperature range was found between 775°C to 800°C. Catalyst with a weight ratio of 2.1

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Synthesis and characterization of N-doped graphene quantum dots-titanium dioxide nanocomposite for photodegradation

Isamar Sarabia Ayala¹

¹National Polytechnic School

Oral
contribution

Abstract

The wide variety of synthetic dyes released by various industries poses a threat to the environment and public health [1]. Most of these dyes possess high water solubility and complex molecular structures which makes it difficult to removed them by conventional methods [2]. In recent years, heterogeneous photocatalysis has proven to be efficient for the treatment of contaminated water. It is based on the generation of reactive species that can rapidly and non-selectively oxidize a wide range of organic pollutants [3]. Titanium dioxide nanoparticles are widely used as a photocatalyst to remove pollutants from wastewater due to their high oxidation power, high surface area, high chemical stability, low toxicity, and low cost [2],[3],[4]. However, their broad band gap (3.02 - 3.2 eV) is a disadvantage for their use in photocatalysis, since the incidence of UV-range photons is required to generate electron-hole pairs by photoexcitation [5]. In the present work, we present the synthesis of N-graphene quantum dots that can improve the photoelectric properties of TiO₂ due to the gain effect on conductivity, up-conversion photoluminescence, and outstanding dye adsorption [6],[7]. N-graphene quantum dots were synthesized

by hydrothermal method and TiO₂ nanoparticles were prepared by sol-gel method. Then NGQDs and TiO₂ mixtures were stirred for 12 h, the solid was separated from the solvent by centrifugation and then dried under vacuum to obtain NGQDs-TiO₂ nanocomposite. The material was characterized using some techniques such as: UV-Vis diffuse reflectance spectroscopy, FT-IR spectroscopy, fluorescence spectroscopy and X-ray diffraction. Adsorption experiments were conducted in the absence of Vis or UV light irradiation. Langmuir and Freundlich models were employed to correlate the experimental adsorption data, and it was found that Freundlich gave better performance in correlating the experimental data for both materials (pure TiO₂ and NGQDs-TiO₂). Photocatalytic activity of both materials was studied by the degradation of methylene blue by UV and Vis light irradiation. Finally, the results showed that N-GQDs can enhanced photoactivity under Vis light irradiation compared to pure TiO₂. NGQDs-TiO₂ nanocomposite exhibits higher adsorption intensity and capacity than non-modified TiO₂ nanoparticles.

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Green Synthesis to produce copper nanoparticles and functionalize with graphene oxide to evaluate antimicrobial activity.

Oral
contribution

Joseth Alejandra Pachacama Ruiz¹, Fabian Ernesto Arias Arias

¹Escuela Superior Politécnica De Chimborazo

Abstract

In the last years, bacteria have been a public health problem, even when antibiotics are one of the alternatives, the long use of them produces bacterial resistance. For this reason, new alternatives have emerged in the nanotechnology field in the last decades, copper nanoparticles and graphene are two of the most interesting materials which had been used in medical application because of antimicrobial properties. In the present work, a nanocomposite of graphene oxide/copper nanoparticles had been synthesized to inhibit *Escherichia coli* and *Staphylococcus aureus* gram negative and gram positive bacteria respectively, which are two bacteria more usual in human population. The synthesis of copper nanoparticles was made by using two reductor reagents copper sulfate pentahydrate and Meyer lemon (*Citrus meyeri*), the graphene oxide was synthesized by Hummer's modified method and the functionalization of copper nanoparticles with graphene oxide were realized by sonication and stirring methods. The evaluation of antimicrobial activity was evaluated by microbiological techniques such as minimum bactericidal concentration (MBC) and minimum inhibitory concentration (MIC). The characterization of graphene, copper nanoparticles and graphene/copper nanoparticles were tested by UV-VIS Spectroscopy, Fourier Transform Infrared Spectroscopy (FTIR), Energy Dispersive X-Ray Spectroscopy (EDS), Scanning Electronic Microscopy (SEM), and Atomic Force Microscopy (AFM). For the seeding of the bacteria, a bacterial dilution of 10^7 was used, which was sown by the agar diffusion technique, and by the dilution technique in broth, the incubation in the two techniques of the bacteria was 37° C. The results showed the MBC of 0.01% for *Escherichia coli* and *Staphylococcus aureus* with a minimum inhibitory concentration of 125 [$\mu\text{g}/\text{mL}$] and 250 [$\mu\text{g}/\text{mL}$], inducing 99.9% of in vitro bacterial death, proposed mechanism behind the good efficiency of graphene/copper nanoparticles in the antimicrobial activity is attributed to the considerable concentration of copper and functional groups in graphene oxide which interacts with the bacterial cell membrane causing cell death.

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Modifications in the structure of graphene films deposited on glass by a 100 eV to 10 keV electron beam

Oral
contribution

Karla Estefanía Moyano Quishpe¹, Cristian Patricio Santacruz Teran¹, Cesar Costa Vera¹, Carlos Reinoso², Beatriz Pérez, Esteban Iribarra¹, Steven Nuñez¹

¹Escuela Politécnica Nacional;²University YachayTech

Abstract

Graphene is a material widely studied for its physical, chemical, and electrical properties; it consists of sp² carbons arranged in hexagons along a two-dimensional lattice [1], [2]. Depending on the method of obtaining it, graphene presents defects within its lattice and harbors impurities, which can be useful in order to functionalize the material for a given application [3]. Several previous works conclude that the structure of graphene can be modified by irradiation with an electron beam. The results of these studies indicate that chemical elements can be added to the graphene lattice after irradiation in a controlled atmosphere, creating bonds that change the carbon hybridization towards sp³ [1], [2], [4], [5]. It is important to point out that the beam can be focused to hit a specific micrometer surface, where the indicated changes are required to occur [6]. In the present study, the effect of irradiation with an electron beam at low energies (1-10 keV) on a graphene film on a glass substrate was analyzed. For this purpose, graphene obtained by an electrochemical method was used. The graphene films were irradiated with an electron

gun with different energy, current, and exposure time, inside a vacuum chamber at a lower pressure of the order of 10⁻⁶ Torr. The samples were characterized before and after irradiation. FTIR spectroscopy was used to observe the functional groups present in the structure, Raman spectroscopy was applied to know the effects on the defect content in graphene, the resistivity of the film was measured by Van der Pauw's method, and the bonds present in the samples were observed by X-ray emitted photoelectron spectroscopy (XPS). The results suggest that the carbon bonds with oxygen decrease in the irradiation process, and new bonds are formed between carbons, causing a reduction process of graphene and forming new bonds between carbons with sp² hybridization.

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Synthesis of silicon oxide nanoparticles using an environmentally friendly approach and their application for the removal of emerging contaminants in aqueous media

Victor H. Guerrero¹, Jennifer Lorena Tejedor Oyos¹

¹Escuela Politécnica Nacional

Oral
contribution

Abstract

Metal oxide nanoparticles have attracted great attention during the last decades because of their potential in catalysis, energy applications and environmental remediation. These nanoparticles are even more attractive if they can be obtained by methods that require relatively low-cost materials and minimize the use of energy

and toxic and expensive reactants [1]. Agricultural residues are particularly interesting as precursors for these nanomaterials, since they are widely available, easy to process, and have low or no cost. Among these residues, rice husk (RH) is one of the most promising. This is due to its high content of silicon, which allows the synthesis of silicon oxide (SiO₂) nanoparticles [2]. Additionally, RH is one of the most abundant residues since it represents 20 wt % of a rice grain and, according to the Food and Agriculture Organization (FAO), the world rice production is set to reach 519 million tons in 2021. On the other hand, RH also constitutes a waste problem in rice-producing regions and the increase of the areas of rice cultivation requires the development of new approaches for their management [3]. In this work, rice husk (RH) was used to synthesize silicon oxide (SiO₂) nanoparticles by a thermal method, following an acid leaching pretreatment. The content of ash, lignin, and hemicellulose in the agricultural residue were determined using ASTM standards. During the synthesis process, the natural precursor was treated with acetic and oxalic acids, and the products obtained were then dried in an oven (100 °C for 24 h) and calcined at 700 °C for 2 h, using a heating rate of 5°C min⁻¹. For the first treatment, acid leaching of RH was performed using a 0.5 M oxalic acid solution under subcritical water conditions (50 bar and 155 °C). For the second treatment, a system without pressure, operating under constant stirring at 95 ± 5 °C, was used for the leaching with a 5 wt % acetic acid solution. The organic acid leaching pretreatments were chosen to reduce the environmental impact of the production of acidic wastes during the conventional inorganic acid treatment using HCl [4]. For comparison purposes, a conventional treatment using a 10 wt % HCl solution was also performed. The silica nanoparticles obtained were characterized by X-ray diffraction (XRD), Raman spectroscopy, dynamic light scattering spectroscopy (DLS), and BET analysis, to study their structure and composition, particle size distribution, and specific surface area, respectively. The diffraction patterns and Raman spectra confirmed the presence of SiO₂. The nanoparticles synthesized were tested to eliminate emerging pollutants such as caffeine (CAF) and triclosan (TCS) from synthetic aqueous solutions. CAF and TCS have been ubiquitously detected in different environmental compartments. Toxicological studies have demonstrated that low concentrations of these contaminants may cause subtle chronic effects on aquatic ecosystems and may pose a risk to human health, due to their possible bioaccumulative effects over long term exposure [5]. The results of batch adsorption tests performed with the nanosilica synthesized using the organic acids showed maximum removal efficiencies of 19.4 ± 3.5% and 50.1 ± 3.7% for CAF and TCS, respectively. The kinetics and adsorption isotherm models that best fitted the data collected were also determined. Finally, we can mention that the results obtained in this work indicate that the silica nanoparticles synthesized by treating rice husk with organic acids are promising candidates for environmental applications, due to their easy processing, adequate and tailorable structural and morphological characteristics, and relatively good adsorptive performance.

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Analysis of the physical mechanism behind the reset transition of HfO₂-based ReRAM devices

Silvana Guitarra¹, Martín Santiago Gavilánez Aguilar¹

¹Universidad San Francisco de Quito

Oral
contribution

Abstract

ReRAM devices are good candidates to be part of a new generation of non-volatile memories due to their favorable characteristics, especially those related to compatibility with CMOS industrial processes [1]. ReRAM devices are simple MIM structures, with two metallic electrodes sandwiching an insulator corresponding to a transition oxide. Its memory concept is based on the resistive switching between two states: Low Resistive State (LRS) and High Resistive State (HRS). The transition from HRS to LRS is called set, while the transition from LRS to HRS is called reset. To be activated, ReRAM devices usually require an electroforming process where oxygen vacancies create a conductive filament (CF) inside the insulator that enables the electrical conduction between the electrodes [2]. Therefore, resistive switching is possible thanks to the CF's local formation (set) or rupture (reset) driven by the applied electric field [3]. In this work, reset switching is investigated with the aim of clarifying the underlying physical mechanism that governs the rupture of the conductive filament. We analyze the reset switching response of the HfO₂-based ReRAM by studying the current-voltage curves on devices of nine different areas: 55x55nm², 65x65nm², 75x75nm², 85x85nm², 105x105nm²,

135x135nm², 1x1um², 3x3um², and 5x5um². The characterized ReRAM devices consist of TiN(30nm)/HfO₂(5nm)/Hf(10nm)/TiN(30nm) stacks with a 1T1R structure. All samples were electroformed with 5mA of compliance current to avoid permanent destruction of the dielectric. Once the CF was formed inside the insulator, the current-voltage characteristics were measured under DC voltage sweep at room temperature. The resultant curves have the typical ReRAM butterfly shape with the already reported cycle-to-cycle variability [4]. In the studied devices, reset transition occurs following two steps. First, at a given reset voltage and current, V_{reset} and I_{reset} , there is an initial CF dissolution step where the conductive filament is disrupted, thus resulting in a transition to an intermediate reset state. During this first transition, the current undergoes a significant decrease, which we quantified with a ΔI . After, there is a smooth but gradual disconnection of the CF whose evidence is the linear IV relationship. After, the ReRAM state changes definitely to HRS when the bias sweep is reversed. To understand the physical mechanism inside the reset process, the statistical analysis of these parameters is presented. In summary, our results show that the conductive filament between nm-size and um-size samples has different sizes. For this reason, the reset process, due to the recombination of oxygen vacancies and ions inside the CF, has the same behavior in both kinds of samples but occurs at different values of current and voltage.

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Photocatalytic activity of compounds obtained from naturally occurring minerals by an environmentally friendly process using pressurized aqueous solutions

Victor H. Guerrero¹, Patricia I. Pontón, Carla Valdivieso²

¹Escuela Politécnica Nacional

Abstract

Photocatalytic compounds are vital in catalytic advanced oxidation processes for wastewater treatment, particularly when processes are driven by the Photo-Fenton reaction that leads to degradation of trace organic chemicals [1]. These compounds are even more attractive if they can be obtained from low cost precursors, by using

energy efficient methods that do not require toxic or expensive reactants. In this work, the photocatalytic activity of an iron oxalate and titanium dioxide obtained by an eco-friendly method that uses ilmenite sands as precursor was investigated. The synthesis was carried out in a reactor in which the ilmenite sands were added to an organic acid aqueous solution for 3 h at 155 °C, 50 bar and 700 rpm. The products obtained were fractionated based on solubility differences and then they were dried at room temperature for 72 h. The resulting powders obtained were characterized by Raman spectroscopy, X-Ray diffraction (XRD), scanning electron microscopy (SEM) and energy dispersive X-ray spectroscopy (EDS). The photocatalytic activity of the extracted compounds was determined against the cationic methylene blue under UV-A radiation (365 nm) for 16 h. Results from Raman and XRD analyses confirmed that the synthesis process designed favored the complete conversion of the ilmenite precursor as define peaks at Raman shifts and 2θ angles corresponding to iron oxalate, titanium dioxide (TiO₂) in anatase form and magnetite were identified [2], [3], [4]. In addition, SEM/EDS analyses showed TiO₂ structures with morphologies that resembled to blunt petals displayed in a spherical fashion with particle sizes smaller than 200 nm, whereas iron oxalate structures were in the submicronic range and of heterogeneous morphology with a rectangular crystal trend. The photocatalytic study showed that methylene blue was indeed photo oxidized under UV-A radiation by the iron oxalate enriched fraction obtained. The photocatalytic mechanism can be attributed to partial N-demethylation of methylene blue to Azure B, as a hypsochromic shift from 662 to 648 nm with a corresponding reduction of the absorbance was observed in the UV spectra [5], [6]. The findings obtained in this study prove that the processing method is a feasible and eco-friendly alternative for obtaining photocatalytic compounds from natural precursors such as the ilmenite sands. The compounds obtained could be potentially used in heterogeneous photo catalysis based on semiconductors (TiO₂) and homogeneous Photo-Fenton processes (Iron (III) oxalate) for drinking and waste water decontamination.

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High-energy physics

Search for invisible Higgs boson decays with vector boson fusion signatures with the ATLAS detector using an integrated luminosity of 139 fb-1

Oral
contribution

Pablo Rivadeneira Bracho¹, O Munir²

¹DESY;²Lehigh Univ

Abstract

Several Beyond Standard Models consider the Higgs boson as the mediator between the Standard Model and Dark Matter. At the LHC, it is possible to probe these Higgs portal Dark Matter models searching for the production of Dark Matter through large values of missing transverse energy generated by the DM particles escaping the detector. Using 139fb⁻¹ of pp collision at a center-of-mass energy of 13 TeV recorded by the ATLAS detector, a search for Higgs bosons produced via vector boson fusion and subsequently decay into invisible particles was developed. The observed number of events was found to be in agreement with the background expectation from the Standard Model. Observed and expected upper limits on the branching fraction of Higgs boson decaying to invisible were derived to be at 0.13 at 95% confidence level. These results were used to set limits on the scattering cross-section of weakly interacting massive particles and nucleons. The invisible decays of additional scalar bosons with masses from 50 GeV up to 1TeV were also studied, and upper limits on the cross section times branching fraction were evaluated to be 0.97 pb for a scalar boson of a mass of 50 GeV, which falls with increasing mass to become 0.12 pb at a mass of 1TeV.

Reference

<https://cds.cern.ch/record/2715447/>

Precision bounds on composite Higgs models at the FCC-ee

Oral
contribution

Andres Pinto¹, Giacomo Cacciapaglia, Aldo Deandrea

¹Université Paris-Saclay

Abstract

A complex scalar field is added to the Standard Model (SM) lagrangian. The influence in the electroweak sector of the new particles arising is studied through the Oblique Parameters in three different scenarios at the FCC-ee. Results showed that it's possible to measure quantum fluctuations for physics beyond the SM.

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Medical physics

Effects of movement artifacts in nuclear hybrid modalities for image diagnostic

Oral
contribution

Pedro Fernando Escudero Villa¹

¹Universidad Tecnológica Indoamerica

Abstract

In diagnostic imaging, hybrid devices integrate two imaging modalities for sequential acquisition, allowing the acquisition of merged images that are valuable tools in diagnostics and treatment. These images combine the information provided by each modality. The image fusion software uses the known positions of the scan table to create the fused image [1]. One of the most common hybrid equipment in Nuclear Medicine services is the SPECT-CT which allows the combination of the metabolic information provided by the volumetric image generated by the gamma camera (that allows the obtention of three-dimensional representations of the radiopharmaceutical distribution in the patient), and by the anatomical information provided by the CT images. The use of phantoms is a common practice in imaging acquisition procedures both for parameter setting and for radiopharmaceutical dosimetry evaluation (phantoms can be of different shapes, sometimes amorphous and with a defined form and unique characteristics, it depends that the body regions and organs that are going to study and analyze) [2], [3]. Additionally, the organ motion produced by

respiratory and cardiac movements is still a significant challenge for the accurate delivery of radiotherapy and diagnostics when using hybrid equipment. Due to the differences in acquisition time of SPECT and CT images (CT has a rapid acquisition in comparison with SPECT) the effect of the patient's respiratory movement on the two acquired imaging modalities will also be different, producing an impact on dosimetry. An example is the treatment of liver tumors by radioembolization [4]. In this treatment, microspheres labeled with ^{90}Y (high-energy beta emitter) are introduced via the femoral route through a catheter. To plan this treatment, a simulation is performed with macroaggregates of albumin (MAA) labeled with Tc-99m to assess the pulmonary shunt and the uptake of the tumor and the healthy liver to be radioembolized. The patient's breathing causes a longitudinal movement of the organs of the abdominal cavity due to the displacement of the diaphragm, which in this case could affect dosimetry.[4], [5] The objective of the present work is to evaluate the effect of movement artifacts caused by the patient's breathing during the acquisition of studies, and to analyze their impact on the fusion of SPECT and CT images. For this propose, we used a PTW L981605 phantom built according to the CEI 61675-1 specific standard for Nuclear Medicine and a QUASAR platform that simulates respiratory movement (14 breaths per minute), on which commercial or self-built phantoms can be placed. The image acquisitions have been made with a filled phantom with Tc-99m (half-life 6.01 h) in different isotopes concentrations to emulate the dosimetry. We systematically evaluated the movement artifacts caused by the patient's breathing during the acquisition of images and their impact on the fusion of SPECT and CT images, considering two aspects, the evaluation of the image register and volume segmentation through the threshold. We found that the phantom movement affects SPECT and CT images in different way compared with works previously published. In the images, we found an artifact related to movement that is not appreciable under the regular condition used to obtain the SPECT images due to the low spatial resolution of this imaging modality. We found an artifact associated with respiratory movement does appear for amplitudes of movement greater than the pixel size of SPECT images, in consequence, the shape of phantom spheres changes in the images acquired. After image processing, we could identify the accuracy of the registration with SPECT and CT images, both for a phantom at rest and for a phantom with simulated respiratory movements.

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Cross calibration of ionization chambers using linear accelerators as a standard to replace isotopic sources and their use for radiotherapy dosimetry

Oral
contribution

Josue Vallejo¹

¹Solca Manabí

Abstract

Traceability, precision, and consistency of radiation measurements are essential in radiation dosimetry, particularly radiation therapy [1]. This work studies the IAEA (International Atomic Energy Organization) document TRS-469 for the calibration of reference dosimeters in external radiotherapy, a document aimed at Secondary Laboratories for Dosimetry Standard (LSED for its initials in Spanish), where the calibration factor of ionization chambers in a high-energy isotopic radiation beam (Co-60) is determined.

In Radiotherapy, it is necessary to calibrate these ionization chambers periodically (recommended every two year) since with these we calibrate our linear accelerators. However, different socioeconomic factors can make this time much longer and it is not always feasible to calibrate all ionization chambers in use.

In this talk, we will study the application of the TRS-469 protocol to develop an in-situ methodology for the cross-calibration of ionization chambers that uses ionization chambers previously calibrated in a secondary laboratory as a starting point. We will talk about the different aspects that influence the determination of this dose [2] and, as these laboratories do not have the high precision equipment needed, we will evaluate the different sources of uncertainty for type A and type B errors [3].

We found that the calibration factor obtained with this methodology is within the expected range of values. This validates the developed methodology for cross-site calibration, together with the error analysis, making it suitable to be used within a quality assurance program.

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Oral
contribution

Shielding assessment in a computed tomography facility

Washington Javier Carrasco Tuston¹

¹Hospital de Especialidades Jose Carrasco Arteaga

Abstract

Computed Tomography CT is currently an effective tool for diagnosing tumors, clots, fractures, internal injuries, bleeding or to guide procedures, biopsies and radiotherapy. CT uses ionizing radiation to generate images, so the safety and radiological protection of the patient and occupationally exposed personnel must be taken into account. The objective of this study is to determine if the secondary barriers of the irradiation room guarantee the protection of the operator and the hospital staff when performing tomographic studies with patients. The calculations are strictly based on the recommendations of report 147 of the National Council for Radiation Protection and Measurements NCRP. It may become more convenient to use the DLP to establish the relevant techniques and to compute shielding requirements directly from DLP rather than CTDI100. The weekly shielding design goal for a controlled area is an air-kerma value of 0.1 mGy week⁻¹. The weekly shielding design goal for an uncontrolled area is an air-kerma value of 0.02 mGy week⁻¹. The Control Room is established as a Controlled Zone. Any physical space adjacent to the Tomography Room is established as a NON-Controlled Zone. To determine the Occupancy Factor, the probability that users will be in the areas surrounding the Tomography Room within a period of one year is considered and this is translated weekly. The Room is surrounded by three corridors so that $T = 1/5$, a Warehouse $T = 1/20$, while for the Floor, the Ceiling and the Control Room $T = 1$. After carrying out the calculations, it is determined that the glass must have an equivalence of 0.89 mm of lead, the control room door must have a sheet of 0.96 mm of lead, the thickness of the ceiling 153.48 mm of concrete and the maximum thickness for the walls turns out to be 147.17 mm of concrete. It is concluded that the existing barriers ensure that the annual dose received in a Controlled Zone and a Non-Controlled Zone do not exceed the established limits of 5 mSv and 1 mSv respectively.

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Comparison between 3D-CRT, IMRT and VMAT techniques for prostate cancer radiation treatment

W V Ona¹

Oral
contribution

¹Radiotherapy Unit, Hospital de Especialidades Carlos Andrade Marin, Quito Av. 18 de Septiembre y Av. Universitaria, Ecuador

Abstract

One of the most important steps related to TPS and the success of IMRT is the optimization process. Main objective is arrive at an optimum intensity pattern through the cost functions. Prostate carcinomas have gone from 3D-CRT to IMRT in radiotherapy with very good results, having a great advantage in avoiding OARs. In the prostate plan, a SIB was used with a prescribed dose of 72 Gy for PTV1 and 63 Gy for PTV2 delivered in 30 fractions. 6 and 10 MV photons commissioned for an Elekta Synergy linear accelerator, equipped with an MLC, were used. Monaco was used as TPS system. The Elekta iViewGT panel was used as the matrix for 2D quality control. Data analysis was done using the conformality index (CI) and the heterogeneity index (HI). A tolerance limit for QC was proposed to be greater than 85%. Step and shoot technique had the highest dose with 74.4 Gy and dMLC plan gave the best D95 (Gy) coverage with 70.3 Gy. On the contrary, the minimum absorbed dose for modulated plans was VMAT and step-and-shoot delivery modes obtained lower values than dMLC. VMAT plan was the best treatment for OARs. Inverse techniques have provided a better plan quality for prostate case. The differences varied among VMAT and dMLC, but they were mainly significant for the target coverage.

Reference

Optics

Oral
contribution

Square metallic shields in photonic crystals

Danny Manuel Calvo Velasco¹
Corporación Universitaria Comfacauca

Abstract

In this work, it is presented the numerical study of 2D photonic crystals (PCs) made of square metallic shields distributed in a square arrangement embedded in air considering the transversal electric (TE) polarization in the $\Gamma - X$ direction. It is presented the modification of the photonic band structure (PBS), which shows the redistribution of bands with low dispersion at lower and higher frequencies around the surface plasmon frequency (SPF) with the decrease in the width of the shield walls. Considering the distributions of the electromagnetic fields in the unitary cell, it is observed high intensity values in the metallic region, even for low frequencies, with a distribution like surfaces plasmons, due to the interaction of the electromagnetic modes located on the inner and exterior shield surfaces. Also, it is observed the distribution of electric field in the inner shield hole at low frequencies, distribution prohibited for the rod geometry, which could be used in technological applications.

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Oral
contribution

Twisted light in vacuum described as a phasor

Erick Lamilla Rubio¹, Manuel Alvarez Alvarado, Peter Iza¹, Arturo Pazmiño Velez
¹Escuela Superior Politecnica del Litoral

Abstract

The Orbital Angular Momentum (OAM) in light beams is a recent explored property with a diverse of perspectives, bringing innovations in the field of optical communications [1], [2], particle manipulation [3], [4] and quantum information [5], [6]. The concept of OAM incorporates chirality and helicity characteristics, which are present in the intrinsic parameters of the light beam such as the wave front and the phase distribution [7], [8]. In this context, OAM of a light beam depends on the spatial distribution of the electromagnetic field and not on the state of polarization of light as reported by Allen et. al [9]. When the angular momentum of the light beam is associated with a wavefront with a helical or twisted shape, the OAM of the beam

is internal and does not depend on the referential origin of the light beam [10]. The helical property presented by the wavefront of a beam with OAM depicts an optical vortex in the centre, that is, the cancellation of the amplitude of the optical wave and the indeterminacy in the spatial distribution of phase at that point [11]. It is relevant to mention that OAM presents optical vortices with a topological integer charge, which determines the number of discontinuities in this phase [12]. Such property has been used for multiplexing with angular orbital moment on communication systems [13], [14], optical encryption [15], quantum sensors [16], [17], lasing generation [18], [19], [20], to mention a few examples. Despite the given applications of optical vortices, a detailed description of the chirality and helicity properties of both the wavefront and the phase distribution for the OAM-bearing beams has not been fully developed to the best of our knowledge. This work presents the description of the phase distribution of a beam with OAM as a helical phase space based on phasor representation (similarly as in electrical circuit theory). An innovative mathematical framework is proposed, which consist in modelling the OAM as a set of helices or petals, which are represented by a rotatory vector that contains the information that describes the nature of the OAM. It is shown that, the basis of this phasor is a helical structure of the phase distribution for the simple model of a beam with OAM that enables to solve complex operations with low computational burden, which can be employed for advanced studies in the field.

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Oral
contribution

Implementation And Testing Of An Optical Tweezers For Capture And Manipulation Of Microparticles

Eugenia Elizabeth Samaniego Onofre¹, Cesar Costa Vera¹

¹Escuela Politécnica Nacional

Abstract

The optical micromanipulation of nano and microparticles is of great current interest. To improve our ability to venture into this area, we have reviewed and assembled the parts of an optical tweezers to achieve the entrapment and manipulation of microparticles in our laboratory. The experimental arrangement combines a beam expansion system $\sim 4X$, a focusing system based on a microscope lens with NA 1.25, combined with an observation system¹. The system focuses the laser beam (658nm) in a very small area to achieve the greatest possible effect on the trapped particles. Changing several times, the assembly system has sought to obtain the main features that the arrangement must present for proper operation such as: alignment of the red laser, collimation of the laser beam, and better focus of the particles¹. As sample, we were used polystyrene microparticles ($2.6\mu\text{m}$). This system allows us to study one of the limit cases: $R \gg \lambda$, where R is the radius of the particles under study and λ the wavelength of the laser used²⁻³. The polystyrene dielectric particles have a refractive index of $n=1.57$. The samples of microparticles were prepared at different concentrations, to decrease spherical aberrations⁴. In addition to the experimental arrangement, we processed the results obtained to obtain the maximum optical trap stiffness of this tool (k) to capture particles using different methods⁵. The results obtained are satisfactory and promising in the area of manipulation and analysis of individual particles. In this presentation, the main challenges and the results obtained will be discussed. The study of the results obtained will allow us to compare with results of other research works in this area.

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Modelling ultrafast laser ablation of aluminum films

Jose Camilo Diaz B¹, Dmitry Ivanov, Gabriel M. Bilmes², Demian Biasetti

¹Universidad Nacional De La Plata;²Centro de Investigaciones Ópticas
(CONICET-CIC-UNLP)

Oral
contribution

Abstract

For a better understanding of the dynamics of laser ablation surface cleaning processes, in this paper we present simulations obtained with a coupled atomistic-continuum computational model, (TTM-MD) of an ultrafast laser ablation process of thin Al films. The ablation of condensed matter under exposure to subpicosecond laser pulses has a number of peculiar properties which distinguish this process from ablation induced by nanosecond and longer laser pulses. At high laser fluences, significantly exceeding the threshold for the melting onset, a collapse of the crystal structure overheated above the limit of crystal stability takes place simultaneously in the whole overheated region within a couple ps, skipping the intermediate liquid-crystal coexistence stage. When the samples are thin films, the dynamics of the relaxation of the laser-induced pressure has an important effect on the temperature distribution. Lattice distortions and stress gradients associated with the relaxation of the laser-induced pressure destabilize the crystal lattice. High tensile stresses generated in the middle of the irradiated film, can also lead to the mechanical disintegration of the sample. In this paper we applied the TTM-MD model with laser pulses of 120 fs at different fluences in order to determine the ablation threshold, and by other hand, to analyze the material and its physical features involved in the laser-matter interaction below the ablation threshold, and then, characterize the ablation process above the ablation threshold.

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Luminescent nanothermometry for biological applications

Luis José Borrero González¹

¹Pontificia Universidad Católica del Ecuador

Abstract

Measuring temperature is of fundamental importance in various technological applications. Thermocouples, thermistors, and infrared thermometers are the most common used for temperature measurements of macroscopic objects. However, if temperature measurements are required in submicroscale systems, these thermometers are not convenient because they are too bulky, for example, to be inserted into cells. In this sense, it is necessary to design new types of thermometers that can be used in this range of scales. In addition, an interest in measuring the temperature of biological systems has grown in the last years. Therefore, biocompatible thermometers are required. On the other hand, luminescent nanothermometry is a non-invasive spectroscopic technique based on the dependence of emission with temperature. The emission parameters that can be temperature dependent are: line-shape of a transition, lifetime, polarization, bandwidth, and luminescence intensity. Different types of materials can be found in the literature as possible thermometers, such as polymers, protein conjugated systems, organic dyes, quantum dots and lanthanide-based materials. Lanthanide-based materials for luminescent nanothermometry are composed of a host material doped with lanthanide ions. Lanthanide ions have interesting optical properties, and their emission spectrum is a fingerprint that is characteristic of each of them. An interesting host material for biological applications is titanium oxide since it does not present toxicity. Temperature sensing through optical materials can be performed by monitoring the fluorescence intensity ratio (FIR) between two different thermally coupled spectral transitions. Recently, we have been studying the spectroscopic properties of titanium oxide nanoparticles doped with europium and neodymium ions. These ions present absorptions and emissions within the first biological window of optical transmission of the tissues. We have also observed that their optical transitions present a strong dependence with temperature in the physiological temperature range, which makes this nanomaterial interesting for the construction of luminescent nanothermometers for biomedical applications.

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TOF MS Spectra simulation for ions from ultrafast and high-field-induced molecular dissociation on the surface of nanoparticles

Oral
contribution

Cesar Costa Vera¹

¹Escuela Politecnica Nacional

Abstract

Aerosolized silica nanoparticles have been demonstrated recently as catalysts in the formation of H₃⁺ via unconventional ways in intense-femtosecond laser [1] using reaction nanoscopy (NanoTRIMS) [2, 3]. This technique is based on three-dimensional ion momentum spectroscopy. Here Time-of-flight Mass Spectrometry (TOF-MS) plays a fundamental role in identifying the molecular fragments generated in the reaction. In this work, with the assistance of the TOF-MS spectra we propose a direct manner for estimating the energy of the adsorbate dissociation reactions occurring in the surface of the nanoparticles. These dissociations are induced by ultrafast pulses through the plasmonic enhancement of the local optical electric fields on the surface of SiO₂, core-shell, and Au-decorated silica nanoparticles with nano-meter resolution. First, we propose suitable space and velocity statistical distributions of putative ions generated on the surface of 300nm spherical particles. The ions are defined on the two poles of the particles, along the polarization direction of the dissociating laser field, with opposite preferred emission directions. Second, the ions are propagated through the geometry of the mass spectrometer by a direct time-of-flight equation. And finally, the generated mass spectra are compared with experimental results on different kinds of nanoparticles. Mechanistic aspects are discussed upon analysis of the results.

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Photonics and the development of immersive virtual environments

Oral
contribution

Daniel Alejandro Loaiza Carvajal¹, María Mercedes Morita², Gabriel M. Bilmes²

¹Centro de investigaciones opticas -CIOp;²Centro de Investigaciones Ópticas (CONICET-CIC-UNLP)

Abstract

Three developments of immersive technologies are presented, each one showing the application of different equipment and algorithms for the creation of virtual environments. First, an augmented reality application to visualize pieces from museum

collections in the Province of Buenos Aires, digitized in 3D through the use of captured reality with photogrammetry. Second, the construction of an imaginary virtual museum using 3D images obtained through captured reality, placing them in a virtual reality application. This museum can be visited using a virtual reality helmet, but it also has a web version and a desktop version. Finally, an application made for the Day of Memory in Argentina, consisting of an intervention in the San Martín square in La Plata, with geolocated augmented reality, which uses GPS to geolocate virtual content over the real world.

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Design And Construction Of A 3D Printed Portable Libs System

Oral
contribution

Omar Oporto Bernal¹, Omar Ormachea, Alex Villazón

¹Universidad Privada Boliviana

Abstract

The present work describes the upgrade of the LIBS prototype designed and built in 2015 at the Universidad Privada Boliviana (UPB), from a Technology Readiness level 4 (TRL4 equipment designed for be used in laboratory) to a Red-line Technology of Level 7 (TRL7 equipment designed for be used in a real environment). To make it possible a new electronic system of control was implemented, based on Arduino and electronic circuits which guarantees a stable laser shooting, separating the circuits based on the voltage used, we were able to extend the useful life of the parts and ensure the firing 100% of the time. The passive Q-switch YAG: Nd+++ laser use a 620 VDC in the main power circuit and a higher pulse of shooting over 10kV. The upgrade consists of the reduce in the size of structures components and improve their resistance, all these components made it in 3D impression, resulting structurally speaking in a more resistant and portable prototype, a pistol with a size 14.5 cm x 18.5 cm x 12 cm and the electrical box with a size of 16.8 cm x 11.8 cm x 11.5 cm. With a functional prototype, tests were carried out to achieve a single pulse in the laser shot with a passive Q-switch scheme, obtaining 600 V as the pertinent voltage in the circuit used, with this configuration, an improvement in the capture of the signal by the spectrometer chamber was obtained. All the designs can be replicated easily with basic electronics components and using a 3D impression.

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-

Teaching of physics

Kolb's Experiential Learning Cycle In The Teaching Of Physics, Particular Thematic: The Archimedes' Principle

Oral
contribution

Byron Giovanni Méndez Puenayán¹

¹Universidad Central del Ecuador

Abstract

The society in its development has different edges to be analyzed, one of them is education, in which the principal objective is to form human beings in scientific and moral aspects. Due to its importance, to better the education systems is a daily task worldwide. In that order of ideas, a big problem shows up, specifically within the teaching and learning processes, which is the students' motivation toward the classes developed. Nowadays, there is little interest shown by the teenagers to attend their schools daily; this, clearly, turns into a routine that, in some cases, may be taken as an obligation. In the concern of what was previously mentioned, it is necessary to find some teaching strategies that would call the students' attention and guarantee their learning; moreover, if the topics of the class are related to the Physics area, in which, in some cases, the topics can become almost impossible to understand in less favorable learning environments. In that context, the current investigation work has the purpose to evaluate the teaching and learning processes done through the methodological use of the Kolb's experiential learning cycle with the Archimedes' principle thematic. The proposed teaching methodology is based on the active, reflexive, theoretical and pragmatic learning styles; having as main premise the variety of learning ways that each person has. In that order of ideas, the Kolb's experiential learning cycle, leaning on the experiential learning, has four class stages which are related to the learning styles previously mentioned and proposed by Peter Honey and Alan Mumford in 1988. The investigation focus has a qualitative character due to the nature of the information that has a relation with the students' behaviors and attitudes during the class process. The CHAE questionnaire was used to gather all the information in which the predominance on each student's learning styles was determined; according to these students, a planning, based on the Kolb's experiential learning cycle, was established. Finally, to find the different outcomes and general

indicators in the context of the class, a field diary and an interview with structured questions were used, where the students redacted their lived experiences, the developed processes, the sensations and emotions obtained on reference to the different activities done; giving answers to questions related to the perception on the development of the teaching and learning process. Such techniques of the information gathering were analyzed with the NVivo program, obtaining the different categories of analysis, in order to study the context units used by the students. The obtained outcomes from the present investigation project denote that: the Kolb's experiential learning cycle generates learnings in a dynamic-participatory class environment in which the different thinking abilities are potentiated, achieving a students' motivation toward science. It is important to notice that to do the teaching process from previous experiences done in the concrete experience of the Kolb's cycle generates an optimum learning environment to stimulate participation abilities, reasoning and creativity, having this way a first approaching to the topic of the class, which then leads to the second stage (reflexive observation) where an analysis of the observed phenomena will be achieved, generating a capacity of observation, comparison and synthesis, allowing the student, in the abstract conceptualization stage, conclude and generalize the topic of the class with the theory proposed, to finally, in the active experimentation, get new applications from the acquired knowledge, involving daily experiences of the thematic. In the same way, in quantitative evaluation terms, an 81, 25% of effectivity was obtained on the evaluation made with the different parameters of the thematic. Finally, it is worth to mention that the 100% of the students get to propose examples or day-to-day applications with the thematic of the class, aspect to be highlighted, because the learning turns significant for each student.

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Coaque, Archeological and Astronomical Museum

Oral
contribution

Jennifer Alexandra Chacón Chávez¹, Ricardo Andrés Caiza Grijalva, Sandra Teresa Procel Guerra, Cristopher Ricardo Erazo Vallejos, Diego S Dominguez¹, Nicolás Vásquez¹, Ana Cabero del Río, Reyes Benítez Pedro Santiago

¹Escuela Politécnica Nacional

Abstract

Coaque, a fishermen village in north coast of Ecuador, is an iconic place in the middle of the world, where archaeology and astronomy converge. Archaeological evidence indicates that since Valdivia (4000-300 BC) and Jamacoaque (700-1450 AD) cultures (Vásquez & Delgado 2012), ancient astronomical knowledge has been represented. Ceramic iconography and stone artifacts depicts the sun, the moon, and the stars and apparently solar calendars used for fishing and agriculture. 16th Century ethnohistorical data is rich on descriptions about the abundance of wealth and land fertility within Equinoctial zones. This awoke the interest of Europeans about the geodesic position (Cieza de León 2005 [1553]:136). Two centuries past until La Condamine and Bouguer of the French-Hispanic Geodesic Mission, first measured the zero degrees latitude at Punta Palmar, just south of Coaque. In that site an inscription for sailors' reference was built (La Condamine 1751:11). Coaque and the nearby region was affected by a 7.8 magnitude earthquake on April 16th, 2016. The event, hit largely urban and rural populations of Manabí, increasing local socio-economic problems (such as education deficit, gender and social inequalities, health and increase of death at birth, environment deterioration, and lack of basic services). The relevance of developing another source for the economic reactivation, based on the rich history of this village, is possible through the project

Coaque, Archeological and Astronomical museum, which aims to contribute with astronomical studies, scientific divulgation and technical workshops for the future creation of this museum. The Escuela Politécnica Nacional (EPN), in association with Escuela Superior Politécnica de Manabí (ESPAM), Universidad San Francisco de Quito (USFQ), Universidad Central (UC), and the leaders of the Coaque community, propose to build an interactive museum combining archaeological and geodesic themes to produce scientific explanations for astronomical phenomena occurring in zero degrees latitude. One of the products of the project is the transit study of emblematic stars of the equinoctial sky, emphasizing in the detectability of high energy galactic sources as the Crab in the TeV range. Other interesting results that emerged from this project is the study of magnetic sands of the beaches near the Equator and the demystification of some wrongpseudo-scientific theories about the phenomena that occur at the zero latitude.

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Other

ON-state reliability of GaN-on-Si Schottky Barrier Diodes: Si₃N₄ vs. Al₂O₃/SiO₂ GET dielectric

Oral
contribution

Eliana Maribel Acurio Méndez¹

¹Escuela Politécnica Nacional

Abstract

In recent years, gallium nitride (GaN) based devices have earned great interest in conversion systems, especially for electronic mid-power applications. GaN technology involves wide bandgap (WBG) material (~ 3.4 eV) yielding high breakdown voltage (~ 3 MV/cm). Furthermore, a 2-D electron gas (2-DEG) quantum well formed at the AlGa_N/GaN heterojunction [1] offers extremely low on-state resistivity. However, one of the greatest challenges remains the reliability [2]. In the case of Schottky-Barrier Diodes (SBDs), the introduction of a gated edge termination (GET) leads to a significant increase in the OFF-state reliability [2]. Only a few works were carried out on the ON-state regime. It is worth reminding that the GET resembles a metal-insulator-semiconductor structure bringing about material compatibility concerns at the semiconductor AlGa_N-barrier/dielectric interface. In-situ defects at this interface may be critical as in MOS-like devices (MOSFET or MOS-HEMT) [3], [4]. Therefore, it is reasonable to apply reliability techniques

(e.g. positive bias temperature instability-PBTI) and metrics like the ones successfully applied to MOSFETs. This work aims to study the reliability of GET-SBDs fabricated on 650-V GaN-on-Si buffers considering single and multilayer dielectrics with different materials. The devices-under-test were processed with either a 45-nm thick PEALD Si₃N₄ dielectric (SiN) or a 35nm PECVD SiO₂ dielectric deposited onto a 2.5nm ALD Al₂O₃ interfacial layer as GET dielectric stack. PBTI experiments were performed under different stress voltages and temperatures. During the stress phase, the devices are biased with a positive anode-to-cathode stress voltage (V_{stress}) ranging between 4V and 7V. To capture the degradation, the stress was interrupted at fixed time intervals (Measure-Stress-Measure technique MSM) up to 1000 s. An I-V curve was measured and compared with the fresh (reference) one to calculate the ON-state threshold voltage shift (ΔV_{TON}), which for these structures is always positive indicating an electron trapping process. After the stress phase, a thermal-de-trapping process (TD) at 300 °C is applied to release the trapped charges during the stress and to prepare devices for subsequent experiments. Weibull distributions fit well the ΔV_{TON} on both sides of the wafer. Similar results were obtained for all experiments. An approximately twice higher degradation is observed on the west side compared to the east side of the wafer, which can be attributed to process-induced variability. From the Weibull distributions, the scale parameter (η) is plotted ($\Delta V_{\text{TON}}_{\eta}$ vs. t_{stress}) for different stress conditions. Large forward stress in the ON-state regime produces ΔV_{TON} shifts in the range of 5 to 100 mV. The data fit well with the model proposed in [4]. The extracted time exponent n exhibits a decreasing behavior with the overdrive stress voltage independently of the dielectric Si₃N₄ or Al₂O₃/SiO₂. The value of the exponent γ about 1 (east side) and 1.15 (west side) suggests the existence of a wide distribution of defect levels centered around the channel Fermi level [4]. This indicates similar accessibility to the dielectric defects in both types of GET dielectrics. Temperature and stress voltage conditions show different reliabilities and variabilities depending on the GET dielectric. For the Si₃N₄ GET-SBDs, the trapped charge density (ΔNOT) is lowered for the east-side devices suggesting a de-trapping phenomenon enhanced by temperature while the west-side devices show the opposite trend. On the other hand, the temperature has a low influence in the trapping and de-trapping process in Al₂O₃/SiO₂ dielectric independently of the side of the wafer. As a result, the Si₃N₄ dielectric produces more trapping phenomena with larger variability than Al₂O₃/SiO₂ devices under the same stress, yet with similar activation energy. The time exponent n is also evaluated as a function of the stress time (so-called trapping rate or b-parameter [3]). The b-parameter measures the evolution of the ratio between the trapping and de-trapping mechanisms under given stress voltage and temperature conditions. It shows important correlations between the ΔNOT increase, the trapping rate, and the variability across the wafer. For the same b-parameter values, ΔNOT is lower for Al₂O₃/SiO₂ compared to Si₃N₄ GET dielectric. In summary, Al₂O₃/SiO₂ dielectric yields better reliability and lower variability across the wafer suggesting a better quality of the AlGa_{0.3}N-barrier/dielectric interface and more uniform process control than with Si₃N₄ dielectric. It makes ALD Al₂O₃/ PECVD SiO₂ dielectric a more attractive option for the 650V AlGa_{0.3}N/GaN SBDs technology.

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Oral
contribution

Study of Hydrogen Sorption/ Desorption Effect on Austenitic Iron-Based Alloys

Katherine Encalada¹, Amarante Böttger

¹Escuela Politécnica Nacional

Abstract

As the requirement of renewable energies alternatives arises, hydrogen has been targeted as an attractive fuel able to contribute to the transition from fossil fuels. The so-called “hydrogen economy” faces the challenge of storage and transport of hydrogen. When talking about storage containers emerge important to study the behavior of the materials for such a purpose. This project is about the study of the surface effect of the interaction between hydrogen with iron-based alloys in the case of 304L stainless steel (uncoated and coated with TiO₂) and Invar alloy. The methodology consisted of electrochemical induced hydrogen evolution on an iron-based austenitic metal cathode taking advantage of the intermediate adsorbates (atomic hydrogen) generated during the reaction to study the electrochemical adsorption efficiency. The characterization of the materials was conducted by techniques like XRF, XRD, optical microscopy, and SEM, before and after hydrogen exposure so that it was possible to evaluate the effect of hydrogen ingress. The results showed that the chemistry of the surfaces is irreversibly changed after the electrochemical induced hydrogen sorption/desorption process due to the formation of oxides. The amounts of hydrogen desorbed were quantified after different H₂ loading times. In all cases, the amount of hydrogen desorbed showed a maximum after which the hydrogen desorbed decreased significantly. The maximum for uncoated 304L stainless steel was after 24 h, 90 min for the coated 304L, and 2 h for Invar. The welds are the most vulnerable sections to hydrogen ingress in both cases. XRD results before hydrogen exposure revealed that 304L consists of an austenitic matrix with around 5% of ferrite. An increment of the austenitic volume fraction of 2.2% was observed after the H₂ sorption/desorption process. Invar is a purely austenitic phase, and no changes in the phase composition were observed after the H₂ sorption/desorption process.

Reference

A full version of the present project, including detailed references, can be found at: Study of Hydrogen Sorption/Desorption Effect on Austenitic Iron-Based Alloys:

Surface Interaction Studied by Cyclic Voltammetry on 304L Stainless Steel and Invar

Relevant sources:

A. V. Uluc, J. M. C. Mol, H. Terryn, and A. J. Böttger. Hydrogen sorption and desorption related properties of pd-alloys determined by cyclic voltammetry. *Journal of Electroanalytical Chemistry*, 734:53–60, 2014. ISSN 15726657. doi: 10.1016/j.jelechem.2014.09.021.

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Dust adhesion physics on photovoltaic surfaces and its application on assisted natural cleaning of solar trackers

Oral
contribution

Giovanni Alejandro Cruz Ortiz¹, Pavel Vorobiev

¹Centro de Investigación en Materiales Avanzados

Abstract

Soiling is a problem that affects the energy production of solar panels by means of two mechanisms, it prevents solar radiation from reaching the photoactive region of the panel and, on the other hand, generates a heating effect on the solar panel, reducing the efficiency of the photovoltaic device and accelerating its degradation. The dust particles are deposited on the surface of the panel by the wind currents. Adhesion occurs due to Van der Waals forces, dependent on the contact area of the tempered glass surface with the dust particle, by gravity due to the mass of the particles, and by capillary forces, which are increased with the amount of humidity, depending on the climate. Desert areas have lower capillary forces than areas with a greater presence of rain. When there is light rainfall or night dew, the dirt adheres more strongly to the panel due to cementation processes and the increase in capillary forces. After the formation of droplets under the conditions with presence of water, the dust that was previously on the surface of the solar panels dissolves in the water droplets, if the rain is not strong enough to make these droplets slide off the panel’s surface, “coffee stains” will be formed in the process of drying. When the water dries, the particles accumulate in the contact line of the drop, depositing mainly in the contact perimeter of the drop. Another problem that limits the energy production of solar panels is the inability to follow the angle of incidence of solar irradiance due to the decoupling that exists between the direction of the incident photons from the sun and the orientation of the fixed solar panels, which most of the time are not pointed at the apparent sun’s position, where the intensity of the sun rays is maximum. To solve this problem, solar trackers have been developed which have the purpose of always pointing an arrangement of solar panels towards the apparent sun’s position. In this project, the positioning capabilities of a solar tracker were used to achieve better assisted natural washing under conditions of weak and heavy rain, using a “passive cleaning” when the rain is intense and an “active cleaning”

when the rain is weak. For passive cleaning, the effect of varying the inclination angle while washing and drying was studied and quantified, analyzing the formation of stains generated by raindrops drying. It was evident that the higher the angle of inclination the greater the effect of gravity on the drops, facilitating their sliding and falling, however, it was found that it is possible to carry out passive cleaning at an angle of inclination that does not require prominent deviation from the angle that fits the position of the sun. In active cleaning, a rocking movement is performed by varying the angle of inclination of the solar tracker with values of $+\theta$ and $-\theta$, which increases the contact time of the raindrops with the surface of the solar panel, allowing a better sweep of dust particles and therefore a more complete washing even in light rain conditions. The experiments showed that the development of solar tracking devices with the ability to generate assisted cleaning taking advantage of the climatic conditions is feasible. Understanding the physics behind soiling, washing, and drying solar panels is critical to improve washing methods.

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Oral
contribution

Radon Indoor Air Pollution

Jheny Orbe Ordoñez¹, Marcella Capua, Gabriela Belén Ureña

¹Escuela Superior Politécnica del Chimborazo

Abstract

Radon (²²²Rn) is a naturally occurring, colorless and odorless radioactive gas that is formed during the decay of uranium-238 isotopes. In its decay process, radon produces radioactive descendants, which adhere to the air and whose inhalation and subsequent deposition and disintegration in the different regions of the respiratory system can cause radiological damage. According to the World Health Organization (WHO), radon is the second cause of lung cancer in the general population, after smoking, being identified as a dangerous air pollutant. Building materials and soil gas that contain radon are the dominant sources of radon indoors. Studies show a

seasonal and day / night variation in radon concentration in houses and buildings. Seasonal variations and the day / night effect are affected by many factors, which vary from country to country. Characteristics of the house, soil and building geology, ventilation practices and climatic conditions are the most important factors. In countries with all four seasons, the minimum radon concentration in summer is typically 40% to 50% of the maximum concentration in winter. This study consisted of determining radon concentrations in the Nuclear Techniques laboratory of the Escuela Superior Politécnica de Chimborazo - Riobamba, in order to evaluate seasonal variations and the day / night effect, in typical conditions of a house in the Ecuadorian Sierra, as well as evaluating the annual average concentration. Measurements were made using a scintillation detector (Lucas Cell) interfaced with the AB7 monitor, manufactured by Pylon Electronics Inc., Canada. Radon monitoring was carried out monthly in 2020, for one week, with measurement intervals of one hour. From the results obtained, the day / night effect on radon concentrations is clearly visible. A markedly different seasonal pattern was evident from that seen in four-season countries. The annual mean concentration was 57 ± 5 Bq m⁻³, a value below the reference level (300 Bq m⁻³) recommended by the European Community in the EURATOM 2013/59 Directive for homes and workplaces.

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Temporal Causality in Quantum Teleportation

Jiri Svozilik¹, Jonnathan Pineda Pineda²

¹Palacký University, Olomouc;²Yachay Tech University

Oral
contribution

Abstract

The development of quantum teleportation protocol [1] has revolutionized the way in which the quantum information transfer is realized, without actually revealing transferred information. In addition, it also offers a new paradigm in the Quantum Computation area [2]. Quantum teleportation makes use of the strangest behaviors that quantum systems can exhibit, related to non-classical non-local correlations, represented by the quantum entanglement, which is indeed necessary to surpass the classical teleportation limit. In our study, we focus on the effect of quantum noise in two basic protocols. The one based on the bipartite entangled states, called the standard quantum teleportation protocol [1,3], and the second one, based on the tripartite entangled states, related to the controlled quantum teleportation [4-6]. Especially, we are interested in the temporal causality when the noise affect above

mentioned protocols in different moments of their execution. For different bipartite and tripartite entangled quantum states we have observed different behaviours, such representing different temporal behaviours of investigated quantum states. In order to verify our theoretical results, we have employed publicly accessible quantum computers of IBM to perform experimental validations, using the Python Qiskit package.

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Design and Construction of a Prototype Machine for Thermoplastic Materials Assembly by Laser Transmission Welding

Oral contribution

Juan Diego Jijón Valdivieso¹, Cesar Costa Vera²

¹Instituto de Investigación Geológico y Energético; ²Escuela Politecnica Nacional

Abstract

A prototype to join thermoplastic materials by laser transmission welding was built in this work. The prototype design is based on the minimum specifications to meet for the study of the welding laser phenomenon, whereby the variables of welding speed and laser output power must be controlled by the machine operator. The construction phase is realized following the drawings obtained from the design phase; with these additionally, the prototype is reproducible and scalable. A computer numerical control – CNC is configured for the laser welding machine, based on the open-source Arduino Platform and the free software Grbl. The laser weld design is converted to G-code to be operated by the machine in the x and y axis. The analyzed variables for laser transmission welding process are welding speed, laser output power and pressure on samples of acrylic material. The prototype was tested with 40 laser welded samples in acrylic with different configurations of the control

variables analyzed in the Universal Testing Machine; whereby, the ultimate tensile strength of the weld zone reached 75 % of the nominal mechanical resistance of the acrylic material. Also, width and deep dimensions of the welded zone were calculated with the aid of digital photographs taken from the absorbent material. In general, tensile strength grows with enlarging the width of the welded zone, but at widths larger than 1 (mm) this strength is reduced back. Finally, simulations of the weld process with laser over the acrylic material were performed, where the heat transfer equation was parametrized as a spherical cap with the width and deep data observed in the sample showing the highest tensile strength. With this, the dynamic heat propagation mechanism of laser transmission welding is illustrated for the acrylic material in the absorbent part.

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Polarization And Biomineralization Of Hydroxyapatite-Barium Titanate Composites

Rafael Uribe¹, Gema Gonzalez, Isamara Rojas, Luis Lascano, Gema Gonzalez

¹Escuela Politecnica Nacional

Abstract

In the search of new materials for bone regeneration, materials with piezoelectric properties look promising. It has been reported that piezoelectric materials induce bone growth and enhance implant integration [1], additionally it has been found that bioactivity increases in negatively charge surfaces such as polarized BaTiO₃ [2] and polarized hydroxyapatite (HAp) [3]. In the present work composites of BaTiO₃-HAp in different compositions were prepared (10/90, 30/70, 50/50, 70/30 and 90/10) by a mixture of nanometric powders and then sintered with and without a steam flow in the range at 1000°C for period of 5 h. The materials were polarized at 130°C, 300 and 400°C applying a dc electric field of 1kV/mm, during for 1 h, the electric field was maintained until the material was cooled down to room temperature. The electric and piezoelectric response were measured immediately after cooling, and then after 1 h and after 24 h. The dielectric measurements of materials were performed at different frequencies (0.1 Hz to 100 KHz). The polarized and unpolarized materials were immersed in simulated body fluid (1.5 SBF) during different periods (from 1 week to 3 weeks). The deposition and growth of hydroxyapatite using the biomimetic method was followed by FTIR, XRD and electron microscopy. The biomineralization process increased with the addition of barium titanate to hydroxyapatite and this effect was greatly improved in the polarized materials. The polarization effect on the crystal growth of hydroxyapatite formed from the SBF solution has been demonstrated. Therefore, these materials look very promising for bone regeneration.

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Synthesis of graphene hydrogel and its application in capacitive deionization

Oral
contribution

Ronny Omar De La Bastida Chiza¹, Leonardo Basile¹

¹National Polytechnic School

Abstract

Water supply has become a serious problem due to population growth. Many technologies such as reverse osmosis (RO), distillation or capacitive deionization (CDI) have been studied to use saltwater as raw material for potable water. CDI is an efficient and low-cost technique in which a porous electrode is used due to its high specific surface area (SSA); carbon materials like active carbon (AC), carbon nanotubes or more recently graphene have been used as versatile electrodes. A three-dimensional graphene porous structure can be prepared by solvothermal methods using graphene oxide or reduced graphene oxide; however, the synthesis of graphene oxide involves strong reagents and a complex process. Here, we show that functionalized graphene hydrogels can be prepared using graphene inks by a solvothermal method. The graphene inks can be prepared by a simpler electrochemical route. The properties and morphology of graphene inks were characterized by spectroscopy and microscopy techniques. The UV-VIS spectroscopy of graphene ink showed a low degree of oxidation, concentrations over 1 mg/ml and efficiency over 25%, the quality of graphene flakes was analyzed using Raman spectroscopy showing an ID/IG ratio over 1 due to the defects of graphene ink, the resistivity was measured by Van der Pauw technique in a film deposited in a glass substrate by drop casting showing a much lower resistivity than graphene oxide, morphology was analyzed using AFM showing an average of lateral size of 1 μm and the numbers of layers between 3 to 6, finally, the specific surface area of graphene flakes was measured using methylene blue adsorption method, resulting in an average specific surface area of 468 m^2/g . Graphene hydrogels electrodes were tested in a two-cell system using cyclic voltammetry, constant current charge discharge, electrochemical impedance spectroscopy showing excellent conductive properties. Cyclic voltammetry showed a capacitive behavior with a rectangular shape and a specific capacitance of 106 F/g at a scan rate of 1 mV/s, constant current charge discharge showed 100% of capacitance retention in 1000 cycles of charge-discharge at a density current of 0.5 A/g. Also, electrochemical impedance spectroscopy analysis showed an inclined line at low frequency derived from electrical double layer capacitance, a series resistance of 1.71 Ω due to the electrolyte resistance and collector-graphene hydrogel interface, a low charge transfer resistance of 2.1 Ω meaning easier ion transfer and a inclined line at low frequency because of Warburg impedance. Finally, salt adsorption capacity was calculated using a single pass experiment with a constant voltage adsorption and constant reverse voltage desorption with a salt capacity adsorption of 16 mg/g at 1.8 V.

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Influence of windy conditions in precipitation particle size distribution corrections in Antisana Region

Oral
contribution

Luis Felipe Gualco Centeno¹, Luis Maisincho, Lenin Campozano¹, Thomas Condom, Marcos Villacís

¹Escuela Politécnica Nacional;

Abstract

The estimation of precipitation in a mountain basin is vital for suitable water management. This task is even more complex in places with temporal snow cover, due to the scarcity of measurements and the strong variations in air temperature (T_a) and wind speed (W_s). Currently, disdrometers have become an alternative device that provides detailed information on precipitation, including diameter size distributions

(DSD), fall velocities that allow to quantify the precipitation type and amount. To improve the measurements in the Antisana area, a Parsivel OTT2disdrometer was installed at 4730 meter above sea level in glacier foreland close to 0°C isotherm was used to study precipitation-type at high-altitude. However, it is known that this device overestimates/underestimates the fall velocity of large/small particles. To overcome these issues, a quality control scheme was applied to remove unrealistic particles, and then shift fall velocities such the mean value match with the diameter-fall velocity relationship of rain, snow, graupel, and hail. A clustering approach was employed to partition the solid precipitation (-SP- if $T_a \leq -1^\circ\text{C}$) and liquid precipitation (-LP- if $T_a \geq 3^\circ\text{C}$) into low, medium, and high WS categories. Corrections were evaluated for light ($\leq 2.62\text{ms}^{-1}$), moderate ($2.62 < W_s \leq 5.92\text{ms}^{-1}$) and high ($> 5.8\text{ms}^{-1}$) wind speed regimes during solid and liquid precipitation events. Filters and corrections affected fast particles with $D < 1\text{mm}$, and particles with $D > 8\text{mm}$ and unrealistically slow fall velocities (1-4) ms^{-1} ; removing around 12% of total particles, especially in high winds where the filters remove 18% and 16% of liquid and solid precipitation particles. In addition, wind increased the collision and breakup frequency increasing small particle concentrations and reducing large particles. Thus, variations of concentration/dispersion and removed hydrometeors were linked with W_s changes. Corrected precipitation, assuming constant density (1g cm^{-3}), gives reliable results for LP with respect to a tipping bucket pluviograph and overestimates SP measured in disdrometer. While corrected precipitation with varying density models achieved fewer differences and better fit respect to both devices. These results improve the knowledge of precipitation microphysics of mountainous tropical zone.

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POSTERS

Astronomy

On the low star formation rate in Sagittarius C

Poster

Karen Marina Martínez Acosta¹

¹Pontificia Universidad Católica de Valparaíso - Universidad técnica Federico Santa María

Abstract

The Central Molecular Zone (CMZ) contains from 3% to 10% of the total molecular gas in the Galaxy, concentrated in turbulent and dense molecular clouds. The star formation rate is low in CMZ, which is an open question since there is a large amount of dense gas clouds where star formation could have started. Sagittarius (Sgr) C is the only known star formation region located in the western side of the CMZ. The main goal of our study was to find out the dominant physical conditions of Sgr C and to study how they could affect the process of star formation in the CMZ. For our study we used archive data obtained with Herschel, Mopra, Nobeyama and NRAO telescopes. We studied the dust emission toward Sgr C using infrared data observed with the Herschel telescope. Using radio data we also studied the kinematic temperature, star formation rate and cloud morphology of Sgr C.

Our study showed a dust temperature of $T_d = 19$ K toward Sgr C, which is in agreement with values estimated in other clouds of the CMZ and the Galactic plane. A high kinetic temperature of ≈ 58 K was determined toward Sgr C, which plays an important role in the cloud fragmentation and subsequent star formation. Based on our radio analysis we found a star formation rate density of $\Sigma\text{SFR} = 4 \times 10^{-3} \text{ Moyr}^{-1} \text{ kpc}^{-2}$ which is lower than that of $\Sigma\text{SFR} = 1000 \text{ Moyr}^{-1} \text{ kpc}^{-2}$ found in LIRGs, which are known high star formation luminous infrared galaxies. Finally, the HCO⁺ emission reveals the presence of cavities and shells in regions where there is no evidence of star formation. These shells could be related to cloud shocks believed to take place in Sgr C. It is thought that cloud shocks may have triggered star formation in other sites of the Galaxy, which is not observed in Sgr C. A comparison between physical conditions in Sgr C with those of high star formation sources allowed to find the parameters that suppress the birth of stars in this Galactic Center region.

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Poster

Simulation of exoplanet spectra to be measured by JWST-LRS-Slitless

BARBIER¹

¹National Polytechnic School

Abstract

Simulation of exoplanet spectra to be measured by JWST-LRS-Slitless Barbier, Hugo¹; Lopez, Ericson^{1,2}; Herrería, David¹; Manzaba, Adrián¹ 1: Escuela Politécnica Nacional, Facultad de Ciencias, Departamento de Física 2: Observatorio Astronómico de Quito (OAQ)

Since 1995, with the first discovery of an exoplanet by M. Mayor and D. Queloz, the science of exoplanets has developed a lot. First, with the multiplication of detection methods, and lately and gradually with characterization techniques. The James Webb Space Telescope (JWST), starting in 2022, will open a new window for the characterization of exoplanet atmospheres. The MIRI instrument, particularly in the LRS-Slitless mode, seems promising to obtain spectra of exoplanets between 4 and 13 micrometers, allowing the detection of gases by transmission spectroscopy, to deduce the abundances of gases such as H₂O, NH₃, CO₂, CO, CH₄, H₂ / He and a temperature-pressure profile (TP), to determine the type of atmosphere of an extra-solar planet. Several simulators have been developed to obtain synthetic spectra of planets, as also for the simulation of telescopes, their modes of operation, and retrieval tools. It is important to have a good understanding of the limits and characteristics of the instruments and tools, in preparation for the study of real data. Knowledge of the telescope's operating modes is essential to obtain an adequate signal-to-noise ratio. The techniques of extraction and treatment of spectra must be well assimilated to extract the maximum information from the spectra obtained. Here, we present our work that focuses on using petitRADTRANS [1] as a simulator to generate transfer or emission spectra of planets, taking into account

characteristics such as: the composition, the T-P profile, the types and distributions of the clouds...Secondly, using MiRISim [2,3] simulator, operating in the MIRI-LRS-Slitless observation mode, the petitRADTRANS synthetic spectra are used in the MIRISim input. These are handled to include the noise generated by the detector itself, cosmic rays ...; and with various recovery tools, we compare the input and output spectra, varying, on the one hand the characteristics of the planetary models and on the other, the observation parameters (number of integrations, frames and observation time)

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On the destruction of shocked clouds in the interstellar medium

Poster

Kevin Josué Imacaña Pozo¹, Wladimir Eduardo Banda-Barragán

¹National Polytechnic School

Abstract

Gas clouds in the interstellar medium are subjected to a variety of dynamical processes. A problem of particular interest to astrophysics is understanding how gas clouds evolve when they are overrun by shocks. As the hot gas sweeps across cold gas clouds, it generates shock waves which can heat up and dissociate cloud gas over short time-scales. This poses serious challenges to our current understanding of cloud acceleration. This project aims at understanding shock heating and acceleration of interstellar clouds. We present numerical simulations of how shocks propagate across interstellar clouds with and without magnetic fields. We show that magnetic fields can change the morphology of interstellar clouds, depending on their orientation with respect to the shock normal. Parallel fields have a little dynamical effect, while perpendicular fields suppress dynamical instabilities.

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Complex systems

Poster

Numerical model of acoustic dispersion around oil wells in Yasuní National Park.

Geoconda Marisela Velasco Castelo¹, Christian Leonardo Vásquez Vega

¹UTA

Abstract

This paper addresses aspects of industrial noise produced by oil extraction facilities in Yasuní National Park, located in the Ecuadorian Amazon, and evaluates its effects on local aerial fauna. It is our hypothesis that acoustic sources within this type of installations could influence the behaviour of wildlife, producing a negative impact on the species. The radial propagation model of acoustic wave propagation in an open field is modified through considerations of geometric divergence attenuation, atmospheric absorption effect and obstacle scattering effects. The measurements made in the field by the research team give us information on atmospheric pressure, temperature, relative humidity and average sound frequency, at different distances from the sources. These data have allowed us to use, for example, the ISO 9613-1 Standard to calculate the absorption coefficient due to atmospheric absorption, as well as the Nord2000 model to take into account the local flora that introduces reflection, dispersion and diffraction phenomena. The results obtained have a scientific, environmental and social impact, due to obtaining conclusive data on the effects of noise caused by the oil industry, and could also serve as a basis for decision-making in the field of environmental regulation, as well as social, with reference to indigenous communities living near oil installations.

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Condensed matter physics

Study Of Modification Of The Inner Surface Of The Hollow Poly-Sulphone Fiber Channels When Irradiated By A Beam Of Electrons With An Energy Of 10 Kev

Poster

Larisa Myshelovka¹, Kristina Vokhmyanina, Artem Pyatigor, Valentina Sotnikova

¹Belgorod National Research University

Abstract

The paper presents the results of a spectral microanalysis of the modified surface of a polysulfine fiber after irradiation with an electron beam with an energy of 10 keV. The studies were carried out by transmission scanning electron microscopy with a dark field detector (HAADF STEM), energy dispersive analysis (EDX), transmission electron microscopy (TEM) and diffraction analysis on a Tecnai Osiris and Tecnai G²30ST microscope at an accelerating voltage of 15 kV. The analysis was carried out on a cross section of the sample. It was found that the inner surface of the channel has a coating, which, as shown by microanalysis data, has a large number of pores, and a plaque spot with a thickness of 400 nm is observed closer to the inner surface of the fiber. The analysis also showed a significant difference in the carbon concentration in the irradiated and unirradiated fiber by 50%. It is possible that such a change in the carbon concentration in the surface layer of the polysulfine fiber will have an impact on the channel capacity in charged particle control studies [1-8].

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Defect Passivation of Hybrid Perovskite Methyl Ammonium Lead Iodide with organic molecules: The 4-tert-butyl pyridine (TBP) molecule case

Poster

Luis Antonio Guallichico Guallichico¹, Matheus Josué Souza Matos¹, Mario Sérgio Carvalho Mazzoni

¹Universidade Federal de Ouro Preto

Abstract

Due to its excellent structural and electronic properties, methylammonium lead iodide perovskite (MAPbI₃) has been one of the most studied in the production of solar cells, which so far has achieved an energy conversion efficiency (ECE) of 25.5% according to NREL. Despite this, the material stability problems still need to be solved through the passivation of defects present in its structure. Lewis base molecules are particularly effective for this task. 4-tert-butyl pyridine (TBP) has been used as

a multifunctional additive that plays a positive role in increasing the photovoltage of materials^{1,2}, but has not yet been tested as a passivator of MAPbI₃ surface. Thus, in this work, the effect of adsorption of pure TBP and addition of Cl-, I- or Br- ions on the slabs surface of orthorhombic perovskites was studied. We employ first-principles calculations based on DFT³ as implemented in the SIESTA⁴ method using conserved norm pseudopotentials in Kleinman-Bylander⁵ factorized form. We use the GGA/PBE6 and vdW-BH7 for the exchange and correlation functional approximation. For real space integrals we use a grid defined by a 350Ry meshcut-off. Initially, 2x1 slabs were tested, onto which a pure TBP molecule and halogen ions were adsorbed. The adsorption of the TBP molecule on the surface of the 2x1 slab (2 layers of PbI₂ and 1 layer of methylammonium iodide (MAI)) in the (010) direction is produced by the bond between the N atom of the TBP and the Pb atom of the slab. The system gap is only 0.03 eV smaller than the system without TBP. The adsorption energy of the TBP to the slab is -0.58 eV. The adsorption of the molecule on the slab leads to an alteration in the DOS peaks in relation to the pristine slab, which can be an indication of probable alterations in the trap states of the surfaces of these slabs. The presence of halogen ions in the 2x1 slab passivated with TBP generates localized states on its surface, which in turn induces a mismatch of its spins. The energy gap is not significantly altered by the presence of the TBP molecule on the surface of a 2x1 slab of MAPbI₃.

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Simulation of Vavilov-Cherenkov X-rays in GEANT4 near the photo absorption edges of carbon

Poster

Dronik Vitaliy¹, Nazhmudinov Ramazan, Kubankin Alexander, Kishin Ivan¹

¹Belgorod National Research University

Abstract

The presented work is devoted to the simulation of Vavilov-Cherenkov X-ray radiation with the GEANT4 package. Appearance of Cherenkov radiation in soft x-ray range has been simulated for carbon target, under different angles of incidence of the primary electrons beam. The effect of Cherenkov cone deformation has been studied.

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-

Poster

Predicting the Mechanical Properties of Borophene by Machine Learning

José Daniel Moreno González¹

¹Escuela Superior Politecnica del Litoral

Abstract

A material of great relevance in the current research context is borophene, a monolayer nanomaterial composed only of boron atoms. Its extraordinary electrical and mechanical properties, similar to those of graphene, have attracted enormous attention from the scientific community (Jiang et al., 2016). At present day, the quality and properties of this kind of nanomaterials are usually detected either experimentally, through first principles calculations, or through simulations. These methods involve a considerable processing complexity and, therefore, a lot of time and resources (Zhang et al., 2019). In addition, a new experiment, simulation or calculation must be carried out each time it is wished to obtain a new result after varying an input parameter. Therefore, the present work proposes to use a model created from a neural network, based on similar previous studies carried out with graphene (Zhang et al., 2019). This model will allow predicting the properties that borophene will present by varying its parameters in a matter of seconds, without performing additional calculations. For the data set gathering stage, the data was collected from molecular dynamics simulations carried out in LAMMPS (LAMMPS Documentation, 2021), an open-source software that allows modeling sets of particles, from atomic systems to more complex systems such as polymers, metallic crystals and other materials in solid, liquid or gaseous state. In this program, a square sheet of borophene of 60 Å each side, corresponding to 1440 boron atoms, was simulated. In these simulations, the Stillinger Weber potential parameterized by Zhou et al. (2017) was used to model the interactions between atoms. Several uniaxial deformation test scenarios were simulated on the material. These scenarios consist of six different temperatures, six strain rates, five initial system speed conditions, and two deformation directions (zigzag and armchair), giving a total of 360 simulations. From each of these simulations, Young's modulus, fracture stress, maximum strain and Poisson's ratio in the direction perpendicular to the plane were obtained. Subsequently, this data set was expanded using a synthetic data generation algorithm based on a Gaussian copula provided by the SDV python library (Patki et al., 2016). As a result, a total of 1440 examples were obtained, of which 20% were separated for the test set, 20% for the validation set and the remaining 60% for the training set. For the design of the neural network, the Keras library

(Keras documentation, n.d.) was used, and a 4-layer architecture was chosen. There is an input layer with three units, one for each input parameter (direction, strain rate and temperature), followed by two intermediate layers, with 20 and 10 units respectively and an output layer with 4 units, one for each value to be predicted (Young's modulus, fracture stress, maximum strain and Poisson's ratio). All units use the ReLU function as the activation function. The training was carried out with 150 iterations or epochs, and the performance was evaluated by means of the mean squared error, resulting in a 0.03% error in the test set. Additionally, a web application with a graphical interface was designed, which uses the trained model, in order to make this tool available to any user. This prototype consists of a simple design, which allows to enter the information corresponding to the parameters required by the user: the strain rate, the temperature and the deformation direction. Once this information has been entered, there is a button that will allow the target values to be displayed on screen.

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Synthesis and electrical properties of MoS₂

Hillary Estefania Rodriguez Lucas¹, Henry Marcelo Osorio Calvopiña¹

¹Escuela Politecnica Nacional

Abstract

Two-dimensional (2D) materials have aroused great interest within various research fields, especially in the manufacture of novel electronic devices. Perhaps the most well-known 2D material is graphene due to its outstanding physical, optical, and mechanical properties; most of them related to its zero band gap. However, in low-power electronics and digital circuits, materials presenting electronic band gaps are also necessary. Transition metal dichalcogenides are interesting compounds that have attracted considerable attention recently because they are atomically thin and exhibit ideal band gaps for electronic and optoelectronic applications. Thus, molybdenum disulphide (MoS₂) is an emerging material due to its unique electronic properties. Contrary to the graphene, MoS₂ shows a band gap which is strongly dependent on the number of layers. Multilayer MoS₂ is an indirect-band-gap semiconductor, with a gap of around 1.2 eV; whilst, the monolayer MoS₂ turns into a direct-band-gap semiconductor with a gap of around 1.8 eV. In this contribution, we describe the use of liquid phase exfoliation technique to obtain MoS₂ nanosheets. Obtained nanosheets are analysed here by using several microscopic and spectroscopic techniques to evaluate their morphology and their chemical and optical properties. Finally, scanning tunnelling spectroscopy is used to evaluate experimentally the electronic band gap of the nanosheets.

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Observation of X-rays during heating a pyroelectric crystal by an infrared laser

Ramazan Nazhmudinov¹, Kubankin Alexander, Andrei Oleinik, Artemiy Klenin

¹Belgorod National Research University

Abstract

The pyroelectric effect has been known for many years and is used for radiation detection, imaging, radiometry and thermometry, energy conversion, etc. [1]. After the publication of Brownridge's work [2], the possibility of using the pyroelectric effect in sources of X-ray and other types of radiation was actively investigated. A commercial miniature X-ray source powered by a 9V-battery has been developed so

far [3]. In all such sources, a pyroelectric crystal located in a vacuum is used as a high voltage generator. The electric potential in this generator is formed when the pyroelectric is heated or cooled. To change the temperature of the crystal, electric heaters or thermoelectric modules are generally used. At the same time, the use of laser radiation can provide better control of the power supplied to the crystal and the heating duration. To date, a prototype of an X-ray source has been proposed [4], in which a lithium niobate crystal is irradiated by an ultraviolet laser through a silica window. We present the results of our experiment on heating a 10 mm thick lithium tantalate crystal by infrared laser radiation with a wavelength of 10 μm , passing into a vacuum chamber through a sodium chloride window. The X-ray spectra measured by the CdTe detector at various values of the heating power and irradiation duration contain bremsstrahlung with an energy of up to 53 keV and characteristic X-rays emitted by the crystal and structural elements of the setup. The work was financially supported by a Program of the Ministry of Education and Science of the Russian Federation for higher education establishments, project No. FZWG-2020-0032 (2019-1569).

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Modifications in flat borosilicate glass samples by electron bombardment in the range of 1 to 10 keV

Poster

Juan De la Torre¹, Steven Nuñez¹, Karla Estefanía Moyano Quishpe¹, Cristian Patricio Santacruz Teran¹, Isamar Sarabia Ayala¹, Esteban Iribarra¹, Cesar Costa Vera¹

¹Escuela Politécnica Nacional

Abstract

The guiding effect is the contactless transmission of charged particles through dielectric materials. It is a phenomenon where the incident beam (ion or electron) forms a charge patch in the dielectric which deflects the beam subsequently [1]. In the experiments carried out by Nguyen et al. [2] using borosilicate glass capillaries, a blue glow was reported during the electron transmission. Additionally, it has been observed on multiple occasions that after a while the channel “gets closed”. That is, the transmission of electrons decreases or disappears suddenly, and this may be related to physicochemical changes of the material. This behavior can be explained by the presence of molecular oxygen on the material’s surface product of electron irradiation [3]. This work presents the modifications in flat borosilicate glass samples after being irradiated by electrons with energies between 1 keV and 10 keV

and beam currents of 10 uA inside a vacuum chamber at 10e-6 Torr. During the irradiation process, a blue glow is observed in the irradiated zone and a gradual decrease in the intensity of the blue glow. After irradiation, a darkening is observed in the impact zone, this phenomenon was quantified by UV-Visible spectroscopy, confirming a decrease in transmittance. The FTIR analysis does not show significant variations between irradiated samples and non-irradiated samples.

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Green synthesis to produce copper nanoparticles using Citrus Meyeri

Poster

Joseh Alejandra Pachacama Ruiz¹, Gabriela Viviana Tubon Usca

¹Escuela Superior Politécnica De Chimborazo

Abstract

Nowadays, copper nanoparticles have a huge scientific interest due to physical, chemical, and biological properties. The copper nanoparticles could be used in medical centers for antimicrobials properties as well as in filler composites, textile, and the cosmetic industry. Hence the importance to propose a green synthesis to obtain copper nanoparticles. In this research work, green synthesis copper nanoparticles were produced using Citrus Meyeri (Limón Meyer) as an acid medium to provoke chemical decomposition of copper sulfate pentahydrate. In order to obtain copper nanoparticles, two methods were carried out. The first one was done using copper sulfate pentahydrate as a precursor in presence of analytic grade ascorbic acid to compare the characteristics and morphology. The second one was in the presence of Citrus Meyeri. In one reaction at 70°C for 1 hour, the coloration change was a preliminary indicator forming nanoparticles. The characterization of nanoparticles was carried out by (UV-vis) Spectroscopy, X Ray Energy Dispersion (EDS), Scanning Electron Microscopy (SEM), infrared transformed Fourier (FTIR) and Atomic Force Microscopy (AFM). The results showed, in a chemical method, a formation of agglomerated nanoparticles in different shape with 70nm and 36% frequency. Meanwhile, the biological synthesis nanoparticles size formed 60 nm and 40% frequency. Finally, the production of copper nanoparticles is 0.77 gr, the biological method can be compared with the chemical or traditional methods, obtaining the similarity in

the reducing agents and an absorbance within the range of 515[nm]. In the EDS analyzes, both methods show the presence of copper. In conclusion, this work offers a green method to produce copper nanoparticles in a simple way with a similar results as chemical method.

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Experimental setup for the study of the interaction of 100 eV – 10 keV electrons with matter

Poster

Steven Nuñez¹, José Luis González peñafiel¹, Juan De la Torre¹, Cristian Patricio Santacruz Teran¹, Esteban Iribarra¹, Cesar Costa Vera¹, Ramon Xulvi-Brunet¹

¹National Polytechnic School

Abstract

An experimental setup to study the interaction of 100 eV – 10 keV electrons with matter was developed. It consists of the electron gun EGG-3101, a vacuum chamber and different detectors. The electron gun has a Tantalum refractory metal disk

which produces an emission current between several nA to 1 mA depending on the applied voltage [1]. It is installed on a cylindrical vacuum chamber of 192 mm radius and 582 mm length which has 4 places to locate the samples being studied. The electrical, mechanical and thermal feedthroughs can be installed in more than 10 KF standard flanges. The geometry allows the execution of different experiments. The vacuum better than 10^{-6} Torr is achieved using an ACP-28 fore vacuum pump and a Hi-Pace 300 turbo molecular pump. The characterization of the electron beam is performed using a Faraday Cup and a ZnS:Ag phosphorus screen. The current is measured by a Keysight 34405A amperemeter. Parameters such the electron energy, divergence, spot size, charge distribution in the beam, and gun alignment were determined. For example, the charge distribution in the beam was measured by installing an aluminium mask with a 1 mm perforation radius in front of the Faraday cup. Then the cup was moved in the direction perpendicular to the electron beam propagation. Studies of the modification of the psico-chemical characteristics of graphene and borosilicate after electron irradiation were performed. Also, the trajectory of the electrons was modified during the interaction of the beam with dielectrics which is called “The guiding effect”. The results of the beam characterization and preliminary studies of the guiding effect are presented in this poster.

Reference

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Poster

Transport Properties of Graphene in proximity with Alkali Metals

Cristina Vaca Chanatasig¹

¹Yachay Tech University

Abstract

The modification of the electronic properties of graphene by depositing adatoms directly on its surface has been achieved experimentally, having potential applications in nanoelectronic devices and being considered a supporting template for catalytic metal particles and energy storage [1]. For instance, the adsorption of alkali metals causes charged impurity scattering on graphene [2], consistent with theoretical predictions [3]. The theoretical models for graphene on alkali metals consist mainly of ab-initio methods based on DFT, which describes their electronic and transport properties [4]. However, these models focus on only one stacking configuration: the hollow site (defined below) [4]. A study of the effects of the adsorption of alkali metals on the transport properties of graphene, taking all the possible sites of adsorption, is essential to understand the storage mechanisms in carbon-based materials for alkali metal batteries [5]. In this project, we propose the analysis of

the transport properties of graphene on alkali metals, such as capacitance, conductance, and currents of charge. We will study three inequivalent metal adsorption sites: the bridge site, above a C–C bond; the top site, on top of a carbon atom of one sublattice of graphene; and the hollow site, in the middle of a C6-unit. In this work, I use an analytical Tight Binding Model (TBM), for graphene with adsorbate atoms of lithium and potassium, in the three different adsorption positions. Then, the Green function calculates the bands and density of state for graphene with adsorbed atoms, and numerical calculations are performed with Kwant, the quantum simulation package of python.

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High-energy physics

A portable particle detector to study natural radioactivity and cosmic rays in open field

Poster

Wilson Santiago Reino Cárdenas¹, Marco Schioppa, Davide Passarelli

¹Università della Calabria

Abstract

In recent years, many particle detectors have been developed and produced for educational purposes. With them it is possible to begin to familiarize with particle detection and pragmatically introduce the word of the infinitely small. Although these detectors are small and have a rate capability di few tens of Hz, they can make very interesting measurements, such as measuring the number of particles per unit of area and time produced by a source, the number of particles after placing a sheet of Pb between the source and the detector, or the water thickness, just to name a few characteristic measures. Some of these measurements can be performed in the open field to find that the natural radioactivity of rocks depends on their chemical composition. The measurements presented here are made with the ArduSiPM particle detector consisting of a 5x5cm tile scintillator, coupled with a silicon photomultiplier readout via an Arduino Due shield. After describing the measurements

made for the characterization of the detector in the laboratory, the measurements made in the open field at different sites with different geologies are described.

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Optics

Poster **Change of temperature in Current Density Gain in Triple Junction Solar Cells with Different Antireflective Coatings**

Darwin Guanga¹, Jaouad Abdelatif, Arnaud Ritou, Maxime Darnon², Hamon Gwénaëlle, Volatier Maïté

¹Sherbrooke University;²Centre national de la recherche scientifique

Abstract

Nowadays, photovoltaic energy is widespread all over the world with the Silicon-based flat panels. Concentrated photovoltaic energy (CPV) uses III-V photovoltaic cells, which absorb in different wavelength ranges of the solar spectrum and reach the highest conversion efficiency of sunlight to electrical energy, up to 47.1% [1]. This work used three triple junction solar cell, (GaInP/GaInAs/Ge), whose have different Anti-Reflective Coatings, SiOx, Bead/PDMS and AlOx/TiOx, respectively, see Figure 1. According to previous results, Short Circuit Current Density Gain (Jsc) of Bead/PDMS respect to 3JSC is 3.7%, it was measured at T=25oC and Irradiance of 900[W/m²] (Indoor condition), by other hand, Jsc is around 6.7% at unknown temperature and Irradiance (Outdoor conditions) [2]. This work aims to understand the difference between indoor and outdoor electrical characterization of different solar cells with different Anti-Reflective Coating, by middle of studying of change of temperature in Short Circuit Current Density Gain and Open Circuit Voltage (Voc). Relation between indoor and outdoor results give the value of unknown temperature in outdoor conditions. The study under indoor conditions was done with EQE and One Sun Simulator techniques in a range of temperatures from 20oC to 45oC. For outdoor condition a previous database of Bead/PDMS and 3JSC was obtained from CPV sub-module adapted at 280X concentration. Results show for indoor data an increasing of Short Circuit Current Density (Jsc) according to temperature in Top sub-cell and keep a constant value for middle sub-cell. For Bead/PDMS

sample, middle sub-cell limits the current. At T=25oC an extra Short Circuit Current Density Gain of Bead/PDMS 3JSC respect to 3JSC was measured, it was attributed to degradation of samples in the time. A comparison between outdoor and indoor measurements shows an increment of short circuit current in temperature for all solar cells even for Bead/PDMS 3JSC, this fact was justified by bad accuracy of the AM1.5D spectrum in the sun simulator. Keywords: Triple Junction Solar Cell, Short Circuit Current Density, Anti-Reflective-Coating, Short Circuit Current Density Gain, EQE, One Sun Simulator, CPV.

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Arduino-Phyton interface for a light photometer

Poster

Carlos Eduardo Smith Rincon¹, Luis José Borrero González², Jesús González-Laprea²

¹Escuela Superior Politécnica del Chimborazo;²Pontificia Universidad Católica del Ecuador

Abstract

The aim of this work is to create an Arduino-Phyton graphical interface for a light photometer. The photometer consists of a light source RGB LED, a light sensor BH1750 and an Arduino Nano microcontroller. The graphical interface can control the turn on and turn off of the LED, control de light intensity, and also read de light sensor. Moreover, the interface can calculate absorbance values. This preliminary prototype has potential to be used in absorption spectroscopy for absorbance measurements of different molecular systems after excitation at three different wavelengths independently.

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Development and Implementation of a Universal Quantum Simulator using the Qiskit platform

Gabriel Cofre¹, Jiri Svozilik²

¹Yachay Tech University; ²Palacký University, Olomouc

Abstract

Can be nature simulated by a computer? The answer is tricky. It would depend on what kind of physics you are treating with, mainly because the way of how information is encoded, processed, and recovered. These are the main differences between classical and quantum computers. Thus, simulating quantum physics with classical computers results usually in the use of a huge amount of computational resources, and an exponential time to solve these kinds of physics systems. As Feynman pointed out in [1], the physical world is quantum, and to simulate it in an "exact" way, we need a computer that behaves exactly the same as Nature does, e.g. quantum computers. Nowadays, there exists a large number of simulations executed on quantum computers based on different physical systems. For instance, the nuclear magnetic resonance (NMR) [2], [3], atoms [4], iontraps [5], and photonic systems [6]. We make use of the quantum circuits approach to implement desired Hamiltonians. The Hamiltonian is split into free (kinetic) and interacting (potential) operators. Meanwhile, the potential term corresponds to a diagonal unitary matrix, to diagonalize the kinetic part, one has to apply the quantum Fourier transformation. Then, the Trotter formula for non-commuting operators is used to approximate the temporal evolution. Nonetheless, this method has some limitations especially for certain systems that need a large number of gates and/or ancillary qubits which dominate the computational resources, such as the proposed in [7]. In our contribution, we develop a universal quantum simulator for quantum systems using the Qiskit platform. It constructs efficient circuits for diagonal unitary operators without ancillary qubits. It has been tested on various potentials and related physical processes.

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Other

how to reduce the pollution produced by motorcycles? : contribution from nanotechnology and materials science

Poster

Jose Fernano Muñoz¹, Jorge Enrique Rodríguez Páez

¹UNIVERSIDAD DEL CAUCA

Abstract

Currently, one of the main problems is the pollution generated by anthropogenic sources that, over time, has been negatively affecting the climate (greenhouse effect), the health of people (respiratory deficits, cancer, among others) and that of animals, in addition to affecting the useful life of different materials. In Colombia, one of the main anthropogenic sources are motorcycles, which are used as transportation and as a means to perform formal and informal work. In this project, nanoparticles were obtained based on ZnO, CeO₂ and MgO, in solid solution with different concentrations, and with them ceramic pieces were formed to which their ability to reduce the amount of polluting gases (CO₂, CO and HC) emitted by mobile sources (motorcycles) was evaluated. The nanocomposites were characterized using X-ray diffraction (XRD) and infrared (IR) spectroscopies - UV-Vis absorption - diffuse reflectance and photoluminescence (PL), as well as high-resolution transmission electron microscopy (HR-TEM). The sintered parts at 700 °C presented a porosity between 11% and 16%, for ZnO-CeO₂, and between 18%-22% for ZnO-MgO, and a grain size of the nanometric order. When these ceramic parts came into contact with the exhaust gases, emitted by the motorcycle, the percentage of gas reduction, considering the obstruction to the exit of the gases by the presence of the piece, was representative. For the different concentrations, the ZnO-(5%)CeO₂ system, reduced HC emissions by 7.5%, CO by 38.21%, and CO₂ by 14.58%, ZnO-(3%) CeO₂, reduced HC emissions by 8.25%, CO by 31.51%, and CO₂ by 5.69% and the ZnO-(1%) CeO₂ system, reduced HC emissions by 11.06%, CO by 12.56% and CO₂ by 3.125%. The ZnO-(5%)MgO system, presented a reduction of 42.99% in the emission of HC, 9.78% in CO₂, the ZnO-(3%)MgO system reduced HC emission by 42.29%, 9.78% in CO₂ and the ZnO-(1%)MgO system presented a 40.22% reduction in HC emission and 2.17% CO₂, being the ceramic piece of ZnO doped at 5% with CeO₂ the one that showed the best result in the reduction of polluting gases.

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A comparative study of liquid-crystal organization in healthy and fatty liver

Poster

María Isabel Subía Potosí¹, Hernán Andrés Morales-Navarrete²

¹Escuela Politécnica Nacional;²University of Konstanz

Abstract

Cell polarity is defined by the patterns that polarity proteins display on cell surfaces (i.e. membrane domains) and it determines a specific cellular structure and function. Simple sheet-like epithelial tissues display single apical and basal domains (i.e. monopoles), therefore, their apico-basal polarity can be defined using a vectorial framework. On the other hand, for more complex three-dimensional tissues, such as liver tissue, the intricate patterns displayed by its membrane domains require a more complex characterization of cell polarity. In 1949, Hans Elias proposed the first structural model describing the organization of hepatic tissue. However, such model does not describe the complex tridimensional organization of the liver. Nowadays, the current development of imaging techniques as well as digital reconstruction methods have allowed scientists to revisit the principles of liver organization with unprecedented accuracy. A conceptual and algorithmic framework to quantify and analyze the spatial patterns of apico-basal hepatic cell polarity in mouse liver tissue was recently developed [1,2]. Using such a framework, it was found that the structure of liver tissue resembles an intermediate state between an amorphous structure and a perfect crystal, best described as a liquid crystal. Considering that previous studies of nematic cell polarity quantification in three-dimensional liver tissue have been performed in murine tissue and that preliminary results showed that liquid-crystalline organizational principles are preserved for tissues of other species, such as human, this study had two main goals: First, further develop and implement computational tools to quantify cell polarity of hepatocytes and apply them to the study of the organization of human liver tissue under two physiologically relevant conditions: healthy tissue and tissue with the pathology of Non-Alcoholic Fatty Liver Disease (NAFLD). Second, elucidate the mechanisms underlying tissue organization (hepatocyte-hepatocyte interactions, boundary conditions, external fields, etc.) using Monte Carlo simulations of liquid crystals in three-dimensional tissue.

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Hearing health virtual assessment through association rules mining inside a college community

Poster

Ruben Alejandro Ortiz Francisco¹, Maria Isabel Subia Potosi, Eliana Maribel Acurio Méndez¹, Hernan Vinicio Barba Molina

¹Escuela Politécnica Nacional

Abstract

This study quantified possible cases of hearing loss and found related factors through association rules mining. The data collection was carried out through an online questionnaire that evaluated general aspects of medical records and the background of the participants, and a free online hearing test provided by the American company Phonak. The sample of this study consisted of 226 entries, among which were students, faculty, and staff members of a public university, the Escuela Politécnica Nacional, from Quito, Ecuador. An Optical Character Recognition algorithm was used for the preliminary data treatment and conversion to binary tables of the audiometry results, implemented through Python. The Apriori algorithm was implemented through the *arules* package for R, to obtain the association rules. Results show that 66.36% of the participants present hearing loss in at least one ear. Additionally, hearing loss in males is primarily related to exposure to loud noises and prolonged use of headphones, and these cases are mostly seen in younger individuals; while hearing loss in females is primarily linked to their family history of deafness.

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Poster

Effect Of Dehydration On The Chlorophyll A Fluorescence Induction: Experiments And Modelling

Erika Quilca¹, Marco Bayas

¹Escuela Politécnica Nacional

Abstract

Chlorophyll a fluorescence induction (FI) is obtained by illuminating dark adapted photosynthetic organisms with photosynthetically active light [1]. In the case of plant leaves, the fluorescence obtained in this way depends on their physiological state. Particularly, stress conditions, such as drought or low temperatures, change the fluorescence vs time curves [2]. Under normal physiological conditions, the fluorescence induction increases from an initial value F_0 to a maximum value F_M exhibiting three clearly differentiated regions, known as OJ (0 - 3ms), JI (3ms - 30ms) e IP (30ms - 300ms) [1, 2]. Here we present a study of the effect of dehydration on the chlorophyll a fluorescence in spinach leaves. The experiments showed that the increase of dehydration moves the curves towards higher values of fluorescence. The F_0 values for all experiments were 1.4 [a.u.] and increased with time to a value of 2.1 [a.u.]. Additionally, when the leaves lost more than 20%

of their masses, the IP regions were absent. To interpret the experimental results, we used a model that associates the fluorescence intensity with both the degree of interconnection between photosystems and with the number of active reaction centers, that is, the ones with the ability to emit fluorescence. The latter depends on the rate of transition between the active and inactive states of each reaction center. Moreover, the model considers that the fluorescence in each region is determined by reaction centers with different kinetics. So the model includes three kinetics constants and three connectivity parameters out of a total of 11. Monte Carlo simulations were used to find the parameters that give the best fit of the theoretical curves to the experimental ones. In this way, the absence of the IP region was explained with the help of the proposed model. It was found that when the IP region was present, the corresponding connectivity parameter increased regularly with time, acquiring values in the range of [0.889-0.991]. This is consistent with the fact that according to the proposed model a connectivity parameter equal to 1 corresponds to the absence of the corresponding region.

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One-step Laser Induced Graphene production for energy storage applications

Poster

Kevin Espinoza¹, Luis Fernando Pantoja, Diego Fierro

¹National Polytechnic School

Abstract

Graphene is a carbon allotrope, which has excellent electrical, thermal, mechanical, chemical and optical properties, giving rise to the investigation of its use in applications such as information storage devices, energy storage devices, electrochemical sensors, photovoltaic devices, among others. [1-3] Despite this, conventional methods to obtain graphene can present problems due to the requirement of precursors, the long time required for processing, the usage of chemicals and / or high temperatures, or high costs. [3-7] In recent years two alternatives have shown up to obtain graphene: Flash graphene and Laser Induced Graphene (LIG). The latter one has advantages over traditional methods, such as not requiring masks or catalysts, as well as being a controllable process that is carried out in a single step. These last two advantages are of great importance for pattern designing in the fabrication of microscale energy storage devices [3]. Among the various energy storage

devices, supercapacitors are shown as a promising alternative to batteries in the portable device market, due to their high power density, long life cycle and fast charge-discharge process [8, 9]. These devices are very promising candidates for applications such as hybrid vehicles and portable electronic devices [10, 11]. The objective of this research is to obtain LIG from a polyimide sheet, using a 450nm CNC laser with a maximum output power of 4.5 W, which will be used for the manufacture of micro-supercapacitors.

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Conformational Transition of Influenza Hemagglutinin Loop-36 Explored with Molecular Dynamics Simulations

Poster

Klever David Cajamarca-Sacta¹, Marco Bayas

¹National Polytechnic School

Abstract

Influenza Hemagglutinin is a protein which undergoes a conformational transition triggered by a pH decrease from 7 to 5. This transition promotes the fusion of the influenza virus to a cell membrane. So, the conformation at pH 7 is called non-fusogenic whereas the one at pH 5 is called fusogenic. A small portion of the protein made of 36 residues, and consequently called "Loop-36" [1], captures the essential features of this transition. The fusogenic and non-fusogenic conformations of Hemagglutinin Loop-36 are well known, but the conformations adopted during the transition have not been completely identified. Here, we report the results of all-atom Targeted Molecular Dynamics (TMD) simulations of loop-36 which allowed us to probe trajectories, in the configuration space, that start in the non-fusogenic conformation and end in the fusogenic one. With a TMD simulation a molecular system is forced to undergo a transition between a initial and a final state by applying an elastic force characterized by an elastic constant k . We performed three TMD simulations with $k = 100, 200$ and 250 [kcal/mol/Å²]. The structures of the three simulations were placed in a single set and a hierarchical agglomerative cluster analysis was performed using the software "R" [2] with the package `proctoclust` [3]. The cluster analysis was done using the euclidean distance and a cut height of 53 angstrom. This height corresponds to a pairwise Root Mean Square Deviation (RMSD) of 2 angstrom which has been defined as a suitable value for a conformation [4]. The resultant clusters were considered to represent preliminary accesible conformations. In order to validate these clusters as representations of "suitable" accesible conformations, the corresponding structures were extensively analyzed and described using general parameters. The first set of parameters used is composed of the first three principal componentes resultant of a Principal Component Analysis (PCA) of the combined structures from the simulations. The second set of paramenters is composed of the Root Mean Square Deviation (RMSD) of each structure, the Radius of Gyration (RGYR), and Fraction of Native Helical Contacts. Our analysis showed that the trajectories correspond to two divergent pathways, in configuration space, followed by the structures en route to the fusogenic conformation. One of the pathways ends in the complete folding of the biomolecule ($k = 200$) whereas the other one ends in an unfolded structure ($k = 100, 250$). This result suggests that the intermediate conformations adopted by Hemagglutinin during its transition from the non-fusogenic to the fusogenic state may not be unique.

Reference

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Poster

Dna Strand Breaks Directly Induced By Kev X-Rays

Andres Ordoñez¹, Marco Bayas

¹National Polytechnic School

Abstract

Nowadays, the quantification of the biological effects of the ionizing radiation used in modern radiodiagnosis is an important objective in basic research because its generalized use has increased the levels of absorbed radiation and consequently, the risks associated on both the patients and the occupational exposed personnel [1, 2]. The risks associated to the low doses deposited by ionizing radiation in radiodiagnosis correspond to the so-called stochastic effects that involve non-lethal damage to the DNA in the cells [1, 2, 3]. This damage can be induced by the presence of high amounts of reactive oxidative species generated by the radiation (indirect damage) [4, 5]. It can also be induced by the direct interaction between the photons and the DNA molecule [4, 5]. Here, we have evaluated the direct damage in the DNA structure caused by keV photons using Monte Carlo simulations. The simulations were done using the Geant4 applications pdb4dna [6] and Geant4-DNA [7, 8] along with an atomically detailed structure of a 347 base pairs DNA molecule. The structure was obtained from the Protein Data Bank [9] and it is part of a di-nucleosome with pdb code 1ZBB. The molecule was irradiated with a monoenergetic photon source uniformly distributed on the surface of a liquid sphere of 16 nm that contains the di-nucleosome. This water sphere simulates the aqueous environment that surrounds the genetic material in living cells. The source emitted one photon at a time towards the interior of the sphere in a random direction. The irradiation was done with photons of 1, 10, 30, 60 and 120 keV. The damage induced in the DNA molecule was quantified with the number of single strand breaks (SSB) and the double strand breaks (DSB) produced in the molecule by each photon. For each energy, the information of 1×10^9 events were collected. Additionally, we studied the dependence between the numbers of strand breaks with the threshold energy required to break the phosphodiester bonds in the DNA strands. The threshold energies were 8, 11, 14, 17 eV. It was found that the number of strand breaks (SSB and DSB) decrease with the energy of the photons according to a potential law whereas it decreases with the threshold energy according to an exponential law. Moreover, the 1 keV photons interacted with the DNA strand with the highest frequency and consequently deposited the highest doses. As a result, these photons had the capacity of producing at least five orders of magnitude more SSBs and six orders of magnitude more DSBs than the 120 keV photons. According to our results,

for the same fluency, the least energetic photons have the capacity of producing the largest amount of strand lesions. However, the number of strand breaks is proportional to the deposited dose in the volume associated to the DNA. Specifically, the numbers of SSB (per Gy and per Gbp) found were 21, 14, 8 and 5 for the threshold energies of 8, 11, 14 and 17 eV, respectively; and the numbers of DSB (per Gy and per Gbp) found were 0.8, 0.3, 0.1 and 0.05 for the threshold energies of 8, 11, 14 and 17 eV, respectively.

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SCHEDULE

MONDAY 25

10:00 - 10:15	INAUGURACIÓN
10:15 - 10:30	Ericson López - Equatorial total electron content
10:30 - 10:45	Camilo Díaz - Modelling ultrafast laser ablation of aluminum films
10:45 - 11:00	Jonathan Quirola - Extragalactic Fast X-ray Transient Candidates Discovered by Chandra
11:00 - 11:15	Ernesto Camacho - ZTF constraints on variability from intermediate-mass black hole candidates
11:15 - 11:30	Wladimir Eduardo Banda Barragán - An overview of shock-multicloud interactions in magnetised galactic winds
11:30 - 11:45	Santiago Arceo Díaz - Evaluation of the survival probability of exoplanets orbiting low-mass stars with enhanced energy loss
11:45 - 12:00	COFFEE BREAK
12:00 - 13:00	Dr. Maarten Boonekamp
13:00 - 14:00	LUNCH
14:00 - 15:00	Dr. Aydogan Ozcan
15:00 - 15:15	COFFEE BREAK
15:15 - 15:30	Pablo Rivadeneira - Search for invisible Higgs boson decays with vector boson fusion signatures with the ATLAS detector using an integrated luminosity of 139 fb ⁻¹
15:30 - 15:45	Andres Pinto - Precision bounds on composite Higgs models at the FCC-ee
15:45 - 16:00	Nicolás Vásquez - Astronomy for development: Astrostays in the middle of the world
16:00 - 16:15	Juan Diego Jijón Valdivieso - Design and Construction of a Prototype Machine for Thermoplastic Materials Assembly by Laser Transmission Welding
16:15 - 16:30	Rafael Uribe - Polarization and biomineralization of hydroxyapatite-barium titanate composites
16:30 - 16:45	Luis Felipe Gualco Centeno - Influence of windy conditions in precipitation particle size distribution corrections in Antisana Region

TUESDAY 26

09:00 - 10:00	Dr. José Vázquez
10:00 - 10:15	COFFEE BREAK
10:15 - 10:30	Danny Manuel Calvo Velasco - Square metallic shields in photonic crystals
10:30 - 10:45	Erick Lamilla Rubio - Twisted light in vacuum described as a phasor
10:45 - 11:00	Eugenia Elizabeth Samaniego Onofre - Implementation and testing of an optical tweezers for capture and manipulation of microparticles
11:00 - 11:15	Luis José Borrero González - Luminescent nanothermometry for biological applications
11:15 - 11:30	César Costa Vera - TOF MS Spectra simulation for ions from ultrafast and high-field-induced molecular dissociation on the surface of nanoparticles
11:30 - 11:45	Daniel Alejandro Loaiza Carvajal - Photonics and the development of immersive virtual environments
11:45 - 12:00	COFFEE BREAK
12:00 - 13:00	Dra. Diana Lopez Tavares
13:00 - 14:00	LUNCH
14:00 - 15:00	Dr. Eric William Burkholder
15:00 - 15:15	COFFEE BREAK
15:15 - 15:30	Omar Oporto Bernal - Design and construction of a 3d printed portable libs system
15:30 - 15:45	Jennifer Alexandra Chacón Chávez - Coaque, Archeological and Astronomical Museum
15:45 - 16:00	Byron Giovanni Méndez Puenayán - KOLB'S experiential learning cycle in the teaching of physics, particular thematic: the archimedes' principle
16:00 - 16:15	Eliana Maribel Acurio Méndez - ON-state reliability of GaN-on-Si Schottky Barrier Diodes: Si ₃ N ₄ vs. Al ₂ O ₃ /SiO ₂ GET dielectric
16:15 - 16:30	Katherine Encalada - Study of Hydrogen Sorption/ Desorption Effect on Austenitic Iron-Based Alloys
16:30 - 16:45	Kevin Espinoza - One-step Laser Induced Graphene production for energy storage applications
16:45 - 17:00	Giovanni Alejandro Cruz Ortiz - Dust adhesion physics on photovoltaic surfaces and its application on assisted natural cleaning of solar trackers
17:00 - 17:15	Ronny Omar De La Bastida Chiza - Synthesis of graphene hydrogel and its application in capacitive deionization

WEDNESDAY 27

08:00 - 12:00	Workshop on Optics
12:00 - 13:00	Dr. Zaidi Habib
13:00 - 14:00	LUNCH
14:00 - 15:00	Dra. Juliana Pavoni
15:00 - 15:15	COFFEE BREAK
15:15 - 15:30	Pedro Fernando Escudero Villa - Effects of movement artifacts in nuclear hybrid modalities for image diagnostic
15:30 - 15:45	Josue Vallejo - Cross calibration of ionization chambers using linear accelerators as a standard to replace isotopic sources and their use for radiotherapy dosimetry.
15:45 - 16:00	William Oña - Comparison between 3D-CRT, IMRT and VMAT techniques for prostate cancer radiation treatment
16:00 - 16:15	Washington Javier Carrasco Tuston - Shielding assessment in a computed tomography facility
16:15 - 16:30	Jheny Orbe Ordoñez - Radon Indoor Air Pollution
16:30 - 18:00	POSTERS

THURSDAY 28

09:00 - 10:00	Dr. Wolfgang Tress
10:00 - 10:15	COFFEE BREAK
10:15 - 10:30	Carlos Reinoso - Catalyst dependency on the growth of single-walled carbon nanotubes
10:30 - 11:45	Galapagos Islands: Virtual tour
11:45 - 12:00	COFFEE BREAK
12:00 - 13:00	Dr. Juan Carlos Idrovo
13:00 - 14:00	LUNCH
14:00 - 15:00	Dr. Bruce Hoeneisen
15:00 - 15:15	COFFEE BREAK
15:15 - 15:30	María José Benítez - Adsorption enhanced photocatalytic degradation of Rhodamine B using GdxBi1-xFeO3@SBA-15 (x= 0, 0.05, 0.10, 0.15) nanocomposites under visible light irradiation
15:30 - 15:45	Rodrigo Sandoval - Electric multipole moments in crystalline insulators
15:45 - 16:00	Jesús González-Laprea - Structural and Thermal Properties of InSb:Mn with MnSb Clusters
16:00 - 16:15	Jimmy Narvárez - Improving the electrical properties of graphene inks by controlling nanosheet thickness distribution
16:15 - 16:30	Esteban Humberto Yépez Jiménez - Electrical characterization of molecular junctions using graphene obtained by electrochemical exfoliation
16:30 - 16:45	Jhonathan Rafael Castillo Saenz - ZnO thin films grown at low temperature by PE-ALD for application in electronic devices
16:45 - 17:00	Jennifer Tejedor - Synthesis of silicon oxide nanoparticles using an environmentally friendly approach and their application for the removal of emerging contaminants in aqueous media
17:00 - 17:15	Carla Valdivieso - Photocatalytic activity of compounds obtained from naturally occurring minerals by an environmentally friendly process using pressurized aqueous solutions

FRIDAY 29

09:00 - 10:00	Dr. Luca Sorriso
10:00 - 10:15	COFFEE BREAK
10:15 - 10:30	Daniela Galárraga Espinosa - Characterising cosmic filaments using hydro-dynamical simulations
10:30 - 10:45	Joseth Alejandra Pachacama Ruiz - Green synthesis to produce copper nanoparticles using Citrus Meyeri
10:45 - 11:00	Joseth Alejandra Pachacama Ruiz - Green Synthesis to produce copper nanoparticles and functionalize with graphene oxide to evaluate antimicrobial activity
11:00 - 11:15	Ramon Xulvi-Brunet - Primary cycles in complex networks
11:15 - 11:30	Esteban Iribarra - Parametric X-ray Radiation from nano meter powders
11:30 - 11:45	Karla Estefanía Moyano Quishpe - Modifications in the structure of graphene films deposited on glass by a 100 eV to 10 keV electron beam
11:45 - 12:00	COFFEE BREAK
12:00 - 13:00	Dr. Vitaly Belik
13:00 - 14:00	LUNCH
14:00 - 15:00	Dr. Konrad Kording
15:00 - 15:15	COFFEE BREAK
15:15 - 15:30	Ramon Xulvi-Brunet - Molecular dynamics algorithm for simulating KeV particles bombardment
15:30 - 15:45	Jilder Dandy Peña Serna - Influence of dopamine on the magnetic properties of superparamagnetic iron oxide nanoparticles
15:45 - 16:00	Rocio Elizabeth Manobanda Guamán - Statistical analysis of pseudo-local properties in turbulent space plasmas using 3d numerical simulations
16:00 - 16:15	Ramon Xulvi-Brunet - Statistical properties of Ecuadorian seismicity
16:15 - 16:30	Lupe Villegas - 3D on-lattice stochastic reaction-diffusion simulation of protein-membrane reversible association
16:30 - 16:45	David Guzmán - Newton-Prygogine y la inter-ciencia
16:45 - 17:15	CLOSURE

E-MAILS

Author	E-mail
A. N. Eliseyev	elisseev@pluton.lpi.troitsk.ru
A.S. Kluev	rinaskela@gmail.com
A.S. Kubankin	kubankin@bsu.edu.ru
Aldo Deandrea	deandrea@ipnl.in2p3.fr
Alexis Debut	apdebut@espe.edu.ec
Amarante Böttger	a.j.bottger@tudelft.nl
Ana Cabero del Río	ana.cabero@epn.edu.ec
Andrés Baquero	jay3guru@gmail.com
Andrei Oleinik	andreyoleynik92@mail.ru
Andres Ordoñez	andres.ordonez@epn.edu.ec
Andres Pinto	andrsp1@hotmail.com
Arnaud Ritou	arnaud.ritou@usherbrooke.ca
Artem Pyatigor	srmemphis322@gmail.com
Artemiy Klenin	starscream046@gmail.com
Arturo Pazmiño Velez	apazmino@espol.edu.ec
Barbier	hugo.barbier@epn.edu.ec
Beatriz Pérez	beatriz.perez@epn.edu.ec
Benjamín Valdez-Salas	berval@uabc.edu.mx
Benjamin Rache Salles	benjamin.rache.salles@gmail.com
Byron Giovanni Méndez Puenay?	byron.mendez@utp.edu.co
Carla Valdivieso	valdivie@ualberta.ca
Carlos Durante	durincarlos@gmail.com
Carlos Eduardo Smith Rincon	carlo1999sr@gmail.com
Carlos Reinoso	creinoso@yachaytech.edu.ec
Cesar Costa Vera	cesar.costa@epn.edu.ec
Christian Leonardo Vásquez Vega	christian.vasquez@epn.edu.ec
Claudio Sangregorio	csangregorio@iccom.cnr.it
Cristian Patricio Santacruz Teran	cristian.santacruz@epn.edu.ec
Cristina Vaca Chanatasig	cristina.vaca@yachaytech.edu.ec
Cristopher Ricardo Erazo Vallejos	cristopher.erazo@epn.edu.ec
Daniel Alejandro Loaiza Carvajal	cohl.daniel@gmail.com
Daniela Galarraga-Espinosa	daniela.galarraga@universite-paris-saclay.fr
Danny Manuel Calvo Velasco	dannycalvo@unicomfauca.edu.co
Darwin Guanga	guad3201@usherbrooke.ca
David Guzmán	dguzman950@puce.edu.ec

David Mateos	david.mateos@uabc.edu.mx
Davide Passarelli	pssdvd98e28d086f@studenti.unical.it
Davide Peddis	davide.peddis@gmail.com
Demian Biasseti	demianb@ciop.unlp.edu.ar
Diego Fierro	diego.fierro@epn.edu.ec
Diego S Dominguez	diego.dominguez@epn.edu.ec
Dmitry Ivanov	ivanov@uni-kassel.de
Dr. Alex Villazón	avillazon@upb.edu
Dr. Omar Ormachea	oormachea@upb.edu
Dronik Vitaliy	dronik@bsu.edu.ru
Eduardo Martínez Guerra	eduardo.martinez@cimav.edu.mx
Eduardo Quintana	evquintanac@gmail.com
Elena Elsa Bricio Barrios	elena.bricio@colima.tecnm.mx
Eliana Maribel Acurio Méndez	eliana.acurio@epn.edu.ec
Erick Lamilla Rubio	ealamill@espol.edu.ec
Ericson López	ericsonl@hotmail.com
Erik Toapanta	erik.toapanta@epn.edu.ec
Erika Quilca	erika.quilca@epn.edu.ec
Ernesto Camacho	eacamacho@uc.cl
Esteban Humberto Yépez Jiménez	stevehyopez@gmail.com
Esteban Irribarra	esteban.irribarra@epn.edu.ec
Eugenia Elizabeth Samaniego Onofre	eugenia94_quito@yahoo.com
Fabian Ernesto Arias Arias	fabian.arias@esepoch.edu.ec
Francisco Servando Aguirre Tostado	servando.aguirre@cimav.edu.mx
Franz Bauer	fbauer@astro.puc.cl
Gabriel Cofre	gabriel.cofre@yachaytech.edu.ec
Gabriel M. Bilmes	gabrielb@ciop.unlp.edu.ar
Gabriela Belén Ureña	gabriela.urena@esepoch.edu.ec
Gabriela Viviana Tubon Usca	gabriela.tubon@esepoch.edu.ec
Gema Gonzalez	ggonzalez@yachaytech.edu.ec
Geoconda Marisela Velasco Castelo	geocovelasco@hotmail.com
Giacomo Cacciapaglia	g.cacciapaglia@ipnl.in2p3.fr
Giovanni Alejandro Cruz Ortiz	giovanni.a.c.o.00@gmail.com
Hamon Gwenaelle	gwenaelle.hamon@usherbrooke.ca
Henry Marcelo Osorio Calvopiña	henry.osorio@epn.edu.ec
Hernán Andrés Morales-Navarrete	hernan.morales-navarrete@uni-konstanz.de
Hernan Vinicio Barba Molina	hernan.barba@epn.edu.ec
Hillary Estefania Rodriguez Lucas	hillary.rodriguez@epn.edu.ec
Isamar Sarabia Ayala	isamar.sarabia@epn.edu.ec
Isamara Rojas	isamara.rojas@epn.edu.ec
Jaime A. Castro	erccastro@yahoo.es
Jaouad Abdelatif	abdelatif.jaouad@usherbrooke.ca
Jennifer Alexandra Chacón Chávez	jennifer.chacon@epn.edu.ec
Jennifer Lorena Tejedor Oyos	jennifer.tejedor@epn.edu.ec
Jesús González-Laprea	jegonzalezl@puce.edu.ec
Jheny Orbe Ordoñez	jenny-orbe@hotmail.com

Jhonathan Rafael Castillo Saenz	jhonathan.castillo@uabc.edu.mx
Jilder Dandy Peña Serna	jilder.pea@gmail.com
Jimmy Narváez	jimmysnarvaez@hotmail.com
Jiri Svozilik	jiri.svozilik@gmail.com
Jonathan Quirola	jaquirola@uc.cl
Jonnathan Pineda Pineda	jonathan.pineda@yachaytech.edu.ec
Jorge Enrique Rodríguez Páez	jnpaez@unicauca.edu.co
José Daniel Moreno González	jdmoreno@espol.edu.ec
José Luis González peñafiel	jose.gonzalez02@epn.edu.ec
Jose R. Fermin	jfermin70@gmail.com
Jose Camilo Díaz B	jcamillo.diazb@gmail.com
Jose Fernando Muñoz	josefmunoz@unicauca.edu.co
Jose Requejo-Isidro	jose.requejo@csic.es
Joseth Alejandra Pachacama Ruiz	pachacama.joseth17@gmail.com
Josue Vallejo	jdvrax@yahoo.es
Juan De la Torre	juan.delatorre@epn.edu.ec
Juan Diego Jijón Valdivieso	judijival@hotmail.com
Kai Zuber	kai.zuber@tu-dresden.de
Karen Marina Martínez Acosta	karen.m91martinez@gmail.com
Karla Estefanía Moyano Quishpe	karla.moyano@epn.edu.ec
Karla Sofia Vizuite Armendáriz	ksvizuite@espe.edu.ec
Katherine Encalada	k.s.encalada@gmail.com
Kevin Espinoza	kevin.espinoza@epn.edu.ec
Kevin Josué Imacaña Pozo	kevin.imacana@epn.edu.ec
Kishin Ivan	ivan.kishin@mail.ru
Klever David Cajamarca-Sacta	kcjprog@gmail.com
Kristina Vokhmyanina	kristinav2005@yandex.ru
Kubankin Alexander	askubankin@gmail.com
Larisa Myshelovka	lareczn@gmail.com
Lenin Campozano	lenin.campozano@epn.edu.ec
Leonardo Basile	leonardo.basile@epn.edu.ec
Luca Sorriso-Valvo	lucasorriso@gmail.com
Luca Sorriso-Valvo	luca.sorriso-valvo@irfu.se
Luis Antonio Guallichico Guallichico	licluisguallichico@gmail.com
Luis Corredor	lcorredor@yachaytech.edu.ec
Luis Felipe Gualco Centeno	luis.gualco@epn.edu.ec
Luis Fernando Pantoja	fernando.pantoja@epn.edu.ec
Luis José Borrero González	ljborrero@puce.edu.ec
Luis Lascano	luis.lascano@epn.edu.ec
Luis Maisincho	lmaisincho@yahoo.com
Lupe Villegas	lupe.villegas@io.cfmac.csic.es
Manuel Alvarez Alvarado	mansalva@espol.edu.ec
Marcela J. Morillo Acosta	marcela.morillo@utc.edu.ec
Marcella Capua	marcella.capua@fis.unical.it

Marcelo Martínez Puente	marcelo.martinez@cimav.edu.mx
Marco Bayas	marco.bayas@epn.edu.ec
Marco Schioppa	marco.schioppa@unical.it
Marcos Villacís	marcos.villacis@epn.edu.ec
María Isael Mendivil Palma	maria.mendivil@cimav.edu.mx
María Mercedes Morita	mercedesm@ciop.unlp.edu.ar
María Isael Subia Potosi	maria.subia01@epn.edu.ec
María Jose Benitez	maria.benitezr@epn.edu.ec
Mario Alberto Curiel Álvarez	mcuriel@uabc.edu.mx
Mario Calixto Rometo Ruiz	mruiz@igepn.edu.ec
Mario Sérgio Carvalho Mazzoni	mazzoni@fisica.ufmg.br
Martín Emilio Mendoza Oliveros	mmendoza76@gmail.com
Martín Santiago Gavilánez Aguilar	msgavilanez@estud.usfq.edu.ec
Martín Albino	martin.albino@hotmail.it
Matheus Josué Souza Matos	matheusmatos@ufop.edu.br
Maxime Darnon	maxime.darnon@usherbrooke.ca
Miguel Novak	mnovak@if.ufrj.br
Nazhmudinov Ramazan	nazhmudinov@bsu.edu.ru
Nicola Nedev	nicolan@uabc.edu.mx
Nicolás Vásquez	nicolas.vasquez@epn.edu.ec
O Munir	na@na.com
Oana Pascu	dr.oanapascu@gmail.com
Omar Oporto Bernal	omar_oportob@hotmail.com
Oscar Perez Landeros	oscar.manuel.perez.landeros@uabc.edu.mx
Pablo Rivadeneira Bracho	pablorb93@gmail.com
Patricia I. Pont??n	patricia.ponton@epn.edu.ec
Paula Sánchez-Sáez	pasanchezsaez@gmail.com
Pavel Vorobiev	pavel.vorobiev@cimav.edu.mx
Pedro Fernando Escudero Villa	pescudero2@indoamerica.edu.ec
Peter Iza	piza@espol.edu.ec
R.M. Nazhmudinov	fizeg@bk.ru
Raúl Puebla	raulpuebla@gmail.com
Rafael Uribe	rafael.uribe@epn.edu.ec
Ramazan Nazhmudinov	ramazan.m.nazhmudinov@gmail.com
Ramon Xulvi-Brunet	ramon.xulvi@epn.edu.ec
Renaud Ferrand	renaud.ferrand@lpp.polytechnique.fr
Reyes Benítez Pedro Santiago	pedro.reyes@epn.edu.ec
Ricardo Andrés Caiza Grijalva	ricardo.caiza@epn.edu.ec
Roberto Andrade	jose.andrade@yachaytech.edu.ec
Rocio Elizabeth Manobanda Guamán	elimanobanda19@gmail.com
Rodrigo Sandoval	rodrigo.sandoval@epn.edu.ec
Ronny Omar De La Bastida Chiza	ronny.delabastida@gmail.com
Ruben Alejandro Ortiz Francisco	ruben.ortiz@epn.edu.ec
Sandra Teresa Procel Guerra	sandra.procel@epn.edu.ec
Santiago Arceo Díaz	santiago.arceo@colima.tecnm.mx
Silvana Guitarra	sguitarra@usfq.edu.ec
Sofia Andrade	sofiacarolina.andradetirado@student.kuleuven.be
Stephen Hernández	hrndz.stphn@gmail.com

Steven Nuñez	steven.nunez@epn.edu.ec
Thomas Cadenbach	tcadenbach@usfq.edu.ec
Thomas Condom	thomas.condom@ird.fr
V. I. Alexeyev	vial@x4u.lebedev.ru
Valentina Sotnikova	levultra@gmail.com
Valeria Ochoa	vochoa@usfq.edu.ec
Victor H. Guerrero	victor.guerrero@epn.edu.ec
Volatier Maíte	maite.volatier@usherbrooke.ca
Washington Javier Carrasco Tuston	wjavierct@gmail.com
Wilson Santiago Reino Cárdenas	wilson.reino.c@gmail.com
Wladimir Benalcazar	wladimir.benalcazar@psu.edu
Wladimir Eduardo Banda-Barragán	wbanda@hs.uni-hamburg.de