



**NSSY2018  
Program**

# **The Nanoscience Summer School @Yachay 2018**

**July 30<sup>th</sup> to August 3<sup>rd</sup> 2018**



# **The Nanoscience Summer School @Yachay 2018 (NSSY) Program**

July 30<sup>th</sup> to August 3<sup>rd</sup> 2018



**SCHOOL OF  
PHYSICAL SCIENCES  
AND NANOTECHNOLOGY**



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San Miguel de Urququí,  
Hacienda San José s/n y Proyecto Yachay  
Telephone: +593 2394 9100

**Organizing Committee:** Duncan John Mowbray  
Henry Paúl Pinto Esparza  
Camilo Zamora Ledezma  
Alicia Mikołajczyk  
Keenan Lyon

### Monday, July 30<sup>th</sup>

#### 9:30 – 10:00 📄 Daily Registration

Sala Capitular

#### 10:00 – 10:30 ▶ Welcome to NSSY2018

Eduardo Ludeña *BSc, MSc, PhD*

Yachay Tech University (Ecuador)

Sala Capitular

#### 10:30 – 11:00 The Roles of Theory, Simulation, and Experiment in Nanoscience

Duncan John Mowbray *BMath, BSc, MSc, PhD*

Yachay Tech University (Ecuador)

Sala Capitular

#### 11:00 – 12:00 Ullmann Coupling of an Inverted Porphyrin on Cu(111): The Role of Cu Adatoms

Juan Carlos Moreno López *BEng, PhD*

University of Vienna (Austria)

Sala Capitular

#### 12:00 – 14:00 ☺ Lunch Break

#### 14:00 – 15:00 Dynamics of Fermions with Periodic Interactions

Alexander Lopez *BSc, MSc, PhD*

Escuela Superior Politécnica del Litoral (Ecuador)

Sala Capitular

#### 15:00 – 15:15 ☕ Afternoon Coffee Break

Sala Capitular

#### 15:15 – 17:00 Workshop 2D Materials: Synthesis, Modifications and Applications for Energy

Damien Voiry *BSc, MSc, PhD*

Institut Européen des Membranes (France)

Sala Capitular

### Tuesday, July 31<sup>st</sup>

#### 9:30 – 10:00 📄 Daily Registration

Sala Capitular

#### 10:00 – 11:00 Graphene and Its Interfaces

Otakar Frank *BSc, PhD*

Czech Academy of Sciences (Czech Republic)

Sala Capitular

#### 11:00 – 11:30 Raman Spectroscopy in Low Dimensional Nanomaterials

Julio Cesar Chacón Torres *BSc, Dr. rer. nat.*

Yachay Tech University

Sala Capitular

#### 11:30 – 12:00 Molecular Dynamics

Alejandro Pérez-Paz *BSc, PhD*

Yachay Tech University

Sala Capitular

#### 12:00 – 14:00 ☺ Lunch Break

Sala Capitular

#### 14:00 – 15:00 Molecular Modeling: Protein-Ligand Docking of Carbon Nanostructures

Bakhtiyor Rasulev *BSc, MSc, PhD*

North Dakota State University (USA)

Sala Capitular

#### 15:00 – 15:15 ☕ Afternoon Coffee Break

Sala Capitular

#### 15:15 – 17:00 Workshop 2D Materials: Electrocatalysis and Nanosieving Applications

Damien Voiry *BSc, MSc, PhD*

Institut Européen des Membranes (France)

Sala Capitular



### Wednesday, August 1<sup>st</sup>

#### 9:30 – 10:00 📄 Daily Registration

Sala Capitular

#### 10:00 – 11:00 Foundations of Density Functional Theory

Eduardo Ludeña *BSc, MSc, PhD*

Yachay Tech University (Ecuador)

Sala Capitular

#### 11:00 – 12:00 Welcome Reception

Eduardo Ludeña *BSc, MSc, PhD*

Yachay Tech University (Ecuador)

Chancellor's Meeting Room

#### 12:00 – 14:00 🍴 Lunch Break

#### 14:00 – 15:00 Using Neural Networks for Approximating Exchange and Correlation Functionals

Keenan Lyon *BSc, MMath*

University of Waterloo (Canada)

Sala Capitular

#### 15:00 – 15:15 ☕ Afternoon Coffee Break

Sala Capitular

#### 15:15 – 15:45 A Multiband Tight-binding Model for Explaining the Rashba+Exchange Effect in Graphene/Au/Co(0001) and Graphene/Co(0001)

Mayra Alejandra de Jesús Peralta Arcia *BSc, MSc, PhD*

Yachay Tech University (Ecuador)

Sala Capitular

#### 15:45 – 16:45 High Performance Computing and Parallelization

Ask Hjorth Larsen *BSc+MSc, PhD*

Universidad del País Vasco UPV/EHU (Spain)

Sala Capitular

### Thursday, August 2<sup>nd</sup>

#### 9:30 – 10:00 📄 Daily Registration

Sala Capitular

#### 10:00 – 11:00 Application of Computational and Cheminformatics Approaches in Toxicity Assessment of Nanomaterials

Bakhtiyor Rasulev *BSc, MSc, PhD*

North Dakota State University (USA)

Sala Capitular

#### 11:00 – 12:00 Computational Design of New and Efficient TiO<sub>2</sub>-Based Photocatalyst: An Environmental Safety Perspective

Alicia Mikołajczyk *BSc, MSc, PhD*

University of Gdansk (Poland)

Sala Capitular

#### 12:00 – 14:00 🍴 Lunch Break

#### 14:00 – 14:30 Hierarchically Structured Materials: From Nanoscale to Macroscale

Gema González Vásquez *BSc, MSc, PhD*

Yachay Tech University (Ecuador)

Sala Capitular

#### 14:30 – 15:00 Magnetic Nanocomposites Decorated with Nanoparticles for Hyperthermia

Sarah Briceño *BSc, PhD*

Venezuelan Institute for Scientific Research (Venezuela) & Yachay Tech University (Ecuador)

Sala Capitular

#### 15:00 – 15:30 📄 Poster Setup

I-103

#### 15:30 – 17:00 📄 Poster Session

I-103

Friday, August 3<sup>rd</sup>

9:30 – 10:00 Daily Registration

Sala Capitular

10:00 – 11:00 Plasmonics in Alkali Metal Intercalated Graphene

Vito Despoja *BSc, MSc, PhD*

Institute of Physics, Zagreb (Croatia)

Sala Capitular

11:00 – 12:00 XPS as an Analytical Tool for the Characterization of Molybdenum Carbide Nanostructures

Joaquín Luis Brito *BSc, MSc, PhD*

Yachay Tech University (Ecuador)

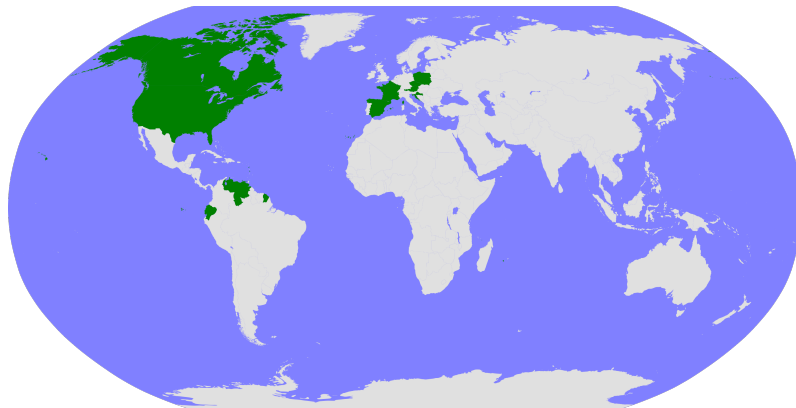
Sala Capitular

12:00 – 12:30 ■ NSSY2018 Closing Remarks

Ernesto Medina Dagger *BSc, PhD, SVG, ICTP-SAIFR*

Yachay Tech University (Ecuador)

Sala Capitular



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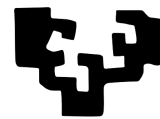


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