



**NSSY2017
Program**

The Nanoscience Summer School @Yachay 2017

August 31st to September 5th 2017



The Nanoscience Summer School @Yachay 2017 (NSSY) Program

August 31st to September 5th 2017





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Editors: Duncan John Mowbray
Henry Paúl Pinto Esparza
Ask Hjorth Larsen
Keenan Lyon

Thursday, August 31st

10:00 – 10:10 ▶ Introduction to NSSY2017
Sala Capitular

10:10 – 11:00 The Roles of Theory, Simulation, and Experiment in Nanoscience
Duncan John Mowbray *BMath, BSc, MSc, PhD*
Yachay Tech University
Sala Capitular

11:00 – 12:00 Molecules on Metals and Graphene: An Experimental Approach
Juan Carlos Moreno López *BEng, PhD*
Yachay Tech University
Sala Capitular

12:00 – 13:00 ☞ Lunch Break

13:00 – 14:00 Molecular Dynamics
Alejandro Pérez-Paz *BSc, PhD*
Yachay Tech University
Sala Capitular

14:00 – 14:15 ☞ Afternoon Coffee Break
I-103

14:15 – 15:15 High Performance Computing and Parallelization
Ask Hjorth Larsen *BSc+MSc, PhD*
Universidad del País Vasco UPV/EHU
I-103

15:15 – 15:30 ☞ Afternoon Coffee Break
I-103

16:00 – 17:00 Cellular Automata
Leonardo Iván Reyes *BEng, MSc, PhD*
Yachay Tech University
Sala Capitular

Friday, September 1st

10:00 – 11:00 Intro to Density Functional Theory
Duncan John Mowbray *BMath, BSc, MSc, PhD*
Yachay Tech University
Sala Capitular

11:00 – 13:00 ☞ Lunch Break
Sala Capitular

13:00 – 14:00 Monte Carlo Methods
Keenan Lyon *BSc, MMath*
University of Waterloo
Sala Capitular

14:00 – 14:15 ☞ Afternoon Coffee Break
Sala Capitular

14:15 – 15:15 Applications of Density Functional Theory
Henry Paúl Pinto Esparza *BSc+MSc, PhD*
Yachay Tech University
Sala Capitular

15:15 – 15:30 ☞ Afternoon Coffee Break
Sala Capitular

17:00 – 20:00 Scientific Python Practicum: Density Functional Hacking
Ask Hjorth Larsen *BSc+MSc, PhD*
Universidad del País Vasco UPV/EHU
I-101

**Monday, September 4th****9:00 – 10:00 Potential Ways to Address the Global Problems: Application of Computational Chemistry**

Jerzy Leszczynski *BSc, MSc, PhD*
Jackson State University
Sala Capítular

10:00 – 10:15 ☕ Morning Coffee Break

Sala Capítular

10:15 – 11:15 Quantitative Structure-Property Relationship Modeling for Surface Modified TiO₂ Based Nanoparticles: Achievements and Perspectives

Alicja Mikołajczyk *PhD*
University of Gdansk
Sala Capítular

11:15 – 12:45 ☕ Lunch Break**12:45 – 13:45 Introductory Raman Lecture**

Jorge Serrano Gutiérrez *BSc+MSc, Dr. rer. nat.*
Yachay Tech University
Sala Capítular

13:45 – 14:00 ☕ Afternoon Coffee Break

Sala Capítular

14:00 – 15:00 Chemical Synthesis of Magnetic Nanoparticles

Sarah Briceño *BSc, PhD*
Venezuelan Institute for Scientific Research & Yachay Tech University
Sala Capítular

15:00 – 16:00 📄 Poster Setup

Library

16:00 – 18:00 📄 Poster Session

Library

Tuesday, September 5th**10:30 – 11:30 An Introduction to Electron Localization Tools in Quantum Chemistry**

Luis Rincon *PhD*
Universidad San Francisco de Quito
Sala Capítular

11:30 – 13:00 ☕ Lunch Break**13:00 – 14:00 Graphene Spectroscopy**

Julio Cesar Chacón Torres *BSc, Dr. rer. nat.*
Yachay Tech University
Sala Capítular

14:00 – 15:00 Graphene Applications

Camilo Zamora Ledezma *BSc, Ph.D.*
Yachay Tech University
Sala Capítular

15:00 – 15:15 ☕ Afternoon Coffee Break

Sala Capítular

15:15 – 16:15 Introduction to Tight Binding

Ernesto Medina Dagger *BSc, PhD, SVG, ICTP-SAIFR*
Yachay Tech University
Sala Capítular

16:15 – 16:30 ■ NSSY2017 Conclusion & Closing Remarks

Sala Capítular