



The Abdus Salam  
International Centre  
for Theoretical Physics



## ICTP Caribbean School on Materials for Clean Energy



Universidad  
de Cartagena  
Fundada en 1827



ACADEMIA COLOMBIANA  
DE CIENCIAS EXACTAS,  
FÍSICAS Y NATURALES



COLCIENCIAS



INSTITUTO DE MATEMÁTICAS APLICADAS



DOCTORADO EN CIENCIAS FÍSICAS

### PROGRAMME

#### Thursday, 30 May 2019

11:00 – 13:30	Morning Session - <i>Campus San Agustín – Of. 330 (Doctorado en Ciencias Físicas)</i>
11:00	<b>Registration &amp; Administrative Formalities 1h0'</b> ( Secretariat )
12:00	<b>Lunch Break 1h30'</b>
13:30 - 17:30	Afternoon Session - <i>Campus San Agustín - Paraninfo Rafael Núñez</i>
13:30	<b>Welcome 30'</b>
14:00	<b>Perovskite Photovoltaics: Computational Modeling 1h0'</b> <i>Speaker: Feliciano Giustino (Oxford University)</i>
15:00	<b>Thermal transport from first principles (Part I) 1h0'</b> <i>Speaker: Stefano Baroni (SISSA/ISAS)</i>
16:00	<b>Coffee Break 30' (3<sup>rd</sup> floor corridor)</b>
16:30	<b>Applications on multiscale computational nanoscience for energy technologies: a pathway towards carbon-neutral cycle 1h0'</b> <i>Speaker: Caetano R. Miranda (São Paulo University)</i>

## Friday, 31 May 2019

08:30 – 14:00

Morning Session - *Campus San Agustín – Aula Máxima de Derecho*

08:30 **Perovskite Photovoltaics: Computational Design** 1h0'  
Speaker: Feliciano Giustino (Oxford University)

09:30 **First-Principles Computations of Reactions at the Electrode/Electrolyte Interface** 1h0'  
Speaker: Perla B. Balbuena (Texas A&M University)

10:30 **Coffee Break** 30' (2<sup>nd</sup> floor corridor)

11:00 **Stacking Fault Energy in Fe-Mn-C alloys: An MD approach** 20'  
Speaker: Manuel Alfonso Camargo Chaparro (U. Antonio Nariño)

11:20 **Controlling novel spin currents in antiferromagnetic materials** 20'  
Speaker: Rafael Julián González Hernández (Uninorte)

11:40 **Thermal transport from first principles (Part II)** 40'  
Speaker: Stefano Baroni (SISSA/ISAS)

12:20 **Lunch Break** 1h30'

14:00 - 17:50

Afternoon Session - *Campus San Agustín – Aula Máxima de Derecho*

14:00 **Thermal transport from first principles (Part III)** 1h0'  
Speaker: Stefano Baroni (SISSA/ISAS)

15:00 **Characterization of photoelectrochemical processes for energy conversion through computer simulations** 1h0'  
Speaker: Nicola Seriani (The Abdus Salam ICTP)

16:00 **Coffee Break** 30' (2<sup>nd</sup> floor corridor)

16:30 **X-ray absorption spectra of Cu and V metal oxides from first principles** 40'  
Speaker: Sebastián Reyes Lillo (U. Andrés Bello)

17:10 **Vibrational properties of germanane and fluorinated germanene in the chair, boat, and zigzag-line configurations** 40'  
Speaker: Jagger Rivera Julio (Centro Atómico de Bariloche)

## Saturday, 1 June 2019

08:30 – 14:00	<p>Morning Session - <i>Campus San Agustín – Aula Máxima de Derecho</i></p> <p><b>08:30 Accelerating Materials Discovery with High-Throughput DFT: The Open Quantum Materials Database (OQMD) 1h0'</b> <i>Speaker: Chris Wolverton (Northwestern University)</i></p> <p><b>09:30 Atomistic classical and quantum simulations of nanobatteries 1h0'</b> <i>Speaker: Jorge Seminario (Texas A&amp;M University)</i></p> <p><b>10:30 Coffee Break 30' (2<sup>nd</sup> floor corridor)</b></p> <p><b>11:00 Understanding Solid-Electrolyte Interface Formation at the Lithium Metal Anode of Lithium-Sulfur Batteries 20'</b> <i>Speaker: Luis Eduardo Camacho Forero (Texas A&amp;M University)</i></p> <p><b>11:20 Vertical Organic Field Effect Transistors based on organic dielectric or electrolyte dielectric materials 20'</b> <i>Speaker: Keli Seidel (U. Tecnológica Federal Do Paraná)</i></p> <p><b>11:40 Rate-limiting step in environmental Bi<sub>2</sub>WO<sub>6</sub> solar light photoelectrocatalysis 40'</b> <i>Speaker: Lorean Mercedes Madriz Ruiz (U. Simón Bolívar)</i></p> <p><b>12:20 Lunch Break 1h30'</b></p>
14:00 – 16:30	<p>Afternoon Session - <i>Campus San Agustín – Aula Máxima de Derecho</i></p> <p><b>14:00 Effects of Applied Potential on Interfacial Reactions 1h0'</b> <i>Speaker: Perla B. Balbuena (Texas A&amp;M University)</i></p> <p><b>15:00 Thermal transport from first principles (Part IV) 1h0'</b> <i>Speaker: Stefano Baroni (SISSA/ISAS)</i></p> <p><b>16:00 Poster parade 30'</b></p>
16:30 – 17:50	<p><b>Poster Session</b> and afternoon snacks c/o <i>Campus La Merced – 1<sup>st</sup> floor corridor</i></p>
17:50 – 21:00	<p><b>Social activity – city tour and school dinner 3h10'</b></p>

## Tuesday, 4 June 2019

08:30 – 14:00	<p>Morning Session - <i>Campus San Agustín – Aula Máxima de Derecho</i></p> <p>08:30 <b>Addressing quantitative or fundamental failures in DFT: Hubbard and Koopmans functionals for energy materials</b> 1h0' <i>Speaker: Nicola Marzari (École Polytechnique Fédérale de Lausanne)</i></p> <p>09:30 <b>Defects and impurity in semiconductors</b> 1h0' <i>Speaker: Eduardo Menéndez (Universidad de Chile)</i></p> <p>10:30 <b>Coffee Break</b> 30' (2<sup>nd</sup> floor corridor)</p> <p>11:00 <b>Physicochemical aspects of the photoelectrocatalysis in nanostructures of Bi<sub>2</sub>WO<sub>6</sub></b> 20' <i>Speaker: David Eduardo Carvajal Guayapero (U. Simón Bolívar)</i></p> <p>11:20 <b>Ultrafast electron dynamics in photoexcited metallic nanoparticles</b> 20' <i>Speaker: Royle Pérez Castillo (Universidad de La Habana)</i></p> <p>11:40 <b>Oxide nanostructures for new concept solar cells: design, morphology control and infiltration under a low cost approach</b> 40' <i>Speaker: Lidice Vaillant Roca ( Universidad de La Habana)</i></p> <p>12:20 <b>Lunch Break</b> 1h30'</p>
14:00 - 17:50	<p>Afternoon Session - <i>Campus San Agustín – Aula Máxima de Derecho</i></p> <p>14:00 <b>Using Artificial Intelligence to Discover New Materials</b> 1h0' <i>Speaker: Chris Wolverton (Northwestern University)</i></p> <p>15:00 <b>Water splitting on hematite (Fe<sub>2</sub>O<sub>3</sub>) surfaces: insights from density-functional theory</b> 1h0' <i>Speaker: Ralph Gebauer (The Abdus Salam ICTP)</i></p> <p>16:00 <b>Coffee Break</b> 30' (2<sup>nd</sup> floor corridor)</p> <p>16:30 <b>Computational Materials Discovery Using the USPEX Code</b> 40' <i>Speaker: Artem Samtsevich (SKOLTECH)</i></p> <p>17:10 <b>Predicting phase transition mechanisms using USPEX code</b> 40' <i>Speaker: Artem Samtsevich (SKOLTECH)</i></p>

## Wednesday, 5 June 2019

08:30 – 14:00	<p>Morning Session - <i>Campus San Agustín – Aula Máxima de Derecho</i></p> <p><b>08:30 <i>Workflows, data, and high-throughput computing for materials discovery 1h0'</i></b> <i>Speaker: Nicola Marzari (École Polytechnique Fédérale de Lausanne)</i></p> <p><b>09:30 <i>Fe-TiO<sub>2</sub> Nanoparticles Synthesized by Green Chemistry for potential Application in Waste Water Photocatalytic Treatment 20'</i></b> <i>Speaker: Ricardo Andrés Solano Pizarro (Unicartagena)</i></p> <p><b>09:50 <i>Monitoring the Applied STRain in Monolayer Gallium Selenide through Vibrational Spectroscopies: A First-Principles Investigacion</i></b> <i>Speaker: Raphael Longuinhos (Universidade Federal de Lavras)</i></p> <p><b>10:10 <i>Closing Remarks</i></b></p> <p><b>10:30 <i>Coffee Break 30' (2<sup>nd</sup> floor corridor)</i></b></p>
11:00 - 17:50	<p>Special activity (<u>requires additional registration on the first day</u>): USPEX tutorial - <i>Campus San Agustín – Computer Room 1<sup>st</sup> floor</i></p> <p><b>11:00 <i>Structural-search code USPEX 6h50'</i></b> <i>Tutors: Artem Samtsevich (SKOLTECH)</i></p>