



The Abdus Salam
International Centre
for Theoretical Physics



Universidad
de Cartagena
Fundada en 1827



ICTP Caribbean School on Materials for Clean Energy

May 30 - June 05, 2019

Cartagena de Indias, Colombia



ACADEMIA COLOMBIANA
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WELCOME TO THE ICTP CARIBBEAN SCHOOL ON MATERIALS FOR CLEAN ENERGY!

Providing abundant amounts of cheap energy is one of the requirements for economic development. Today, mainly fossil fuels are converted to heat and electricity, with only minor contributions from nuclear or hydroelectric sources.

The concomitant production and release into the atmosphere of CO_2 in vast quantities is the main reason for the observed and accelerating change of climate. The global mean temperature is continuously rising, and the goal to limit global warming to 1.5 to 2 degrees requires a complete de-carbonization of the world's economies in the coming few decades. This is obviously a formidable task.

Providing similar amounts of cheap energy as it is obtained today by using fossil fuels, but in a clean and still cost-effective way is probably the most important challenge which materials science is facing today.

Why materials science? Because the most abundant, but diffuse and intermittent clean energy sources are solar light and wind. And to convert those sources into economically useful energy forms (electricity, chemical fuels), functional materials are needed: solar photovoltaic materials, new catalysts or battery materials are just a few examples.

In this school, we aim to illustrate some of those materials-science related issues and to present some promising new solutions. We will also introduce you to how atomistic computer simulations can play an important role on our path towards a cleaner and more sustainable future.

We hope you will all enjoy this school and discover some concrete ideas about how you can gear your own research activities towards our common goal of constructing a clean future for all.

– The Directors

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SCHOOL PROGRAM

Venue:	P. Rafael Núñez	Aula Máxima de Derecho			
Schedule	Thu, May 30	Fri, May 31	Sat, Jun 1	Tue, Jun 4	Wed, Jun 3
08:30 - 09:30		KL-04	KL-09	KL-13	KL-17
09:30 - 09:50		KL-05	KL-10	KL-14	ST-07
09:50 - 10:10					ST-08
10:10 - 10:30					Closing Remarks
10:30 - 11:00		Coffee Break	Coffee Break	Coffee Break and Group Picture	Coffee Break
11:00 - 11:40	Registration	ST-01	ST-03	ST-05	Optional USPEX Hands On
11:40 - 12:20		ST-02	ST-04	ST-06	
12:20 - 13:30		KL-06	IT-03	IT-04	
13:30 - 14:00	Opening	Lunch	Lunch	Lunch	
14:00 - 15:00	KL-01	KL-07	KL-11	KL-15	Lunch
15:00 - 16:00	KL-02	KL-08	KL-12	KL-16	Optional USPEX Hands On
16:00 - 16:30	Welcome Snack	Coffee Break	Poster Parade	Coffee Break	
16:30 - 17:10	KL-03	IT-01	Poster Session (La Merced)	IT-05	
17:10 - 17:30		IT-02		IT-06	
17:30 - 17:50	Tourist Info and City-walls Walk		Social Event		
18:00 - 19:30					
19:30 - 21:00					

KL – Keynote Lecture: 60 Minutes (50 + 10)

IT – Invited Talk: 40 Minutes (30 + 10)

ST – Short Talk: 20 Minutes (15 + 5)

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KEYNOTE LECTURES

FELICIANO GIUSTINO (OXFORD UNIVERSITY – UK)	
KL-01	Perovskite Photovoltaics: Computational Modeling
KL-04	Perovskite Photovoltaics: Computational Design
STEFANO BARONI (SISSA – ITALY)	
KL-02	Thermal transport from first principles (Part I)
KL-06	Thermal transport from first principles (Part II)
KL-07	Thermal transport from first principles (Part III)
KL-12	Thermal transport from first principles (Part IV)
CAETANO R. MIRANDA (SÃO PAULO UNIVERSITY – BRASIL)	
KL-03	Applications on multiscale computational nanoscience for energy technologies: a pathway towards carbon-neutral cycle
PERLA BALBUENA (TEXAS A&M UNIVERSITY – USA)	
KL-05	First-Principles Computations of Reactions at the Electrode/Electrolyte Interface
KL-11	Effects of Applied Potential on Interfacial Reactions
NICOLA SERIANI (THE ABDUS SALAM ICTP – ITALY)	
KL-08	Characterization of photoelectrochemical processes for energy conversion through computer simulations
CHRIS WOLVERTON (NORTHWESTERN UNIVERSITY – USA)	
KL-09	Accelerating Materials Discovery with High-Throughput DFT: The Open Quantum Materials Database (OQMD)
KL-15	Using Artificial Intelligence to Discover New Materials
JORGE SEMINARIO (TEXAS A&M UNIVERSITY – USA)	
KL-10	Atomistic classical and quantum simulations of nanobatteries
NICOLA MARZARI (EPFL – SWITZERLAND)	
KL-13	Addressing quantitative or fundamental failures in DFT: Hubbard and Koopmans functionals for energy materials
KL-17	Workflows, data, and high-throughput computing for materials discovery
EDUARDO MENÉNDEZ (UNIVERSIDAD DE CHILE – CHILE)	
KL-14	Defects and impurity in semiconductors
RALPH GEBAUER (THE ABDUS SALAM ICTP – ITALY)	
KL-16	Water splitting on hematite (Fe_2O_3) surfaces: insights from density-functional theory



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INVITED TALKS

IT-01	SEBASTIÁN REYES LILO (UAB – CHILE)
	X-ray absorption spectra of Cu and V metal oxides from first principles
IT-02	JAGGER RIVERA JULIO (CAB – ARGENTINA)
	Vibrational properties of germanane and fluorinated germanene in the chair, boat, and zigzag-line configurations
IT-03	LOREAN MERCEDES MADRIZ RUIZ (USB – VENEZUELA)
	Rate-limiting step in environmental Bi_2WO_6 solar light photoelectrocatalysis
IT-04	LIDICE VAILLANT ROCA (U. DE LA HABANA – CUBA)
	Oxide nanostructures for new concept solar cells: design, morphology control and infiltration under a low-cost approach
IT-05	ARTEM SAMTSEVICH (SKOLTECH – RUSSIA)
	Computational Materials Discovery Using the USPEX Code
IT-06	ARTEM SAMTSEVICH (SKOLTECH – RUSSIA)
	Predicting phase transition mechanisms using USPEX code



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SHORT TALKS

ST-01	MANUEL ALFONSO CAMARGO CHAPARRO (UAN – COLOMBIA)
	Stacking Fault Energy in Fe-Mn-C alloys: A MD approach
ST-02	RAFAEL JULIAN GONZÁLEZ HERNÁNDEZ (UNINORTE – COLOMBIA)
	Controlling novel spin currents in antiferromagnetic materials
ST-03	LUIS EDUARDO CAMACHO FORERO (TEXAS A&M UNIVERSITY – USA)
	Understanding Solid-Electrolyte Interphase Formation at the Lithium Metal Anode of Lithium-Sulfur Batteries
ST-04	KELI SEIDEL (U. TECNOLÓGICA FEDERAL DO PARANÁ – BRASIL)
	Vertical Organic Field Effect Transistors based on organic dielectric or electrolyte dielectric materials
ST-05	DAVID EDUARDO CARVAJAL GUAYAPERO (USB – VENEZUELA)
	Physicochemical aspects of the photoelectrocatalysis in nanostructures of Bi ₂ WO ₆
ST-06	ROYLE PÉREZ CASTILLO (UNIVERSIDAD DE LA HABANA – CUBA)
	Ultrafast electron dynamics in photoexcited metallic nanoparticles
ST-07	RICARDO ANDRÉS SOLANO PIZZARRO (UNICARTAGENA – COLOMBIA)
	Fe-TiO ₂ Nanoparticles Synthesized by Green Chemistry for Potential Application in Waste Water Photocatalytic Treatment
ST-08	RAPHAEL LONGUINHOS (UNIVERSIDADE FEDERAL DE LAVRAS – BRASIL)
	Monitoring the Applied Strain in Monolayer Gallium Selenide through Vibrational Spectroscopies: A First-Principles Investigation

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POSTERS

P-01	RAPHAEL LONGUINHOS (UNIVERSIDADE FEDERAL DE LAVRAS – BRASIL)
	Stable holey two-dimensional C ₂ N structures with tunable electronic structure
P-02	LUZ MARY RAMÍREZ MONTES (UNINORTE – COLOMBIA)
	Properties of new two-dimensional materials of group VI
P-03	YULISSA RAMÍREZ (UNICARTAGENA – COLOMBIA)
	Synthesis of TiO ₂ nanoparticles co-doped with N-Fe to be used in the water photoelectrolysis
P-04	DAVID SERVELLON CARPIO (NATIONAL SCIENCE RESEARCH CENTER OF EL SALVADOR – EL SALVADOR)
	Synthesis of nanoparticles by microemulsion
P-05	WILFREDO ORTEGA OCHOA (UNICARTAGENA – COLOMBIA)
	Photocatalytic degradation of fungicides used in cocoa crops in the Montes de María region applying heterogeneous solar photocatalysis with CoFe ₂ O ₄ /TiO ₂ nanoparticles
P-06	GUSTAVO RAMIREZ CABALLERO (UIS – COLOMBIA)
	Effect of Defect-Engineering on Microporous/Mesoporous MOF-808 Textural, Surface, and Acidic Properties
P-07	SERGIO G. CONEJEROS ESPÍNDOLA (U. CATÓLICA DEL NORTE – CHILE)
	Non-polar GaP- ZnS nanofilms for photocatalytic applications: A computational approach
P-08	ISMAEL ANTONIO GONZÁLEZ RAMIREZ (UNICOR – COLOMBIA)
	A DFT study about the effects of exchange-correlation functional on the structural and electronic properties of Anatase
P-09	VICTOR MENDOZA ESTRADA (UNINORTE – COLOMBIA)
	Electronic structure and magnetic order in Cu _x Zn _(1-x) O: An ab-initio study
P-10	MARTHA INÉS ORTIZ TORRES (UNIANDES – COLOMBIA)
	Strategies for the set up and characterization of the photoconductive response in photo electrochemical hybrid devices based on graphene and light harvesting proteins
P-11	JHON FABER ZAPATA CARDONA (U. DE SAN MARTÍN – ARGENTINA)
	Electroreduction of CO ₂ on LaBaCoO Perovskites

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P-12	ISAAC VILLALOBOS GUTIÉRREZ (UNIVERSIDAD DE COSTA RICA - CR)
	A study of electric properties in Graphene and Borophene β 12 nanoribbons
P-13	HENRY ANDRÉS CORTÉS PÁEZ (CNEA – ARGENTINA)
	Li_2O_2 formation on CeO_2 catalysts in lithium–oxygen batteries
P-14	ESTEBAN DAVID GADEA (U. DE BUENOS AIRES – ARGENTINA)
	Modelling of surface nanobubbles
P-15	FLORENCIA EMILSE LURGO (U. NACIONAL DE CÓRDOBA – ARGENTINA)
	Magnetization reversal in mixed perovskites with cation Lu^{3+} on the a-site
P-16	FELIPE BARRÍA CÁCERES (UNIVERSIDAD DE CHILE – CHILE)
	Modeling the interaction of fullerene derivatives with hybrid perovskite surface
P-17	LUCAS NICOLAS LODEIRO MORAGAS (UNIVERSIDAD DE CHILE – CHILE)
	Alignment of bands in $\text{Cu}_2\text{O}/\text{CH}_3\text{NH}_3\text{PbI}_3$ interfaces
P-18	MARÍA GABRIELA CAMPOS F. (UNIVERSIDAD DE COSTA RICA – CR)
	DFT computational study of Erythrite
P-19	JESÚS EDUARDO CASTELLANOS ÁGUILA (U. DE GUANAJUATO – MEXICO)
	Theoretical band alignment for an hyperdoped material $\text{CuAlSe}_2/\text{CuGaS}_2$: Cr/ZnSe
P-20	MÓNICA OLEA AMEZCUA (B.U. AUTÓNOMA DE PUEBLA – MEXICO)
	Effects of electron doping on the stability and superconductivity of alkali-metal hydrides without applied pressure: an ab-initio study
P-21	ARLES VICTOR GIL REBAZA (NATL. U. OF LA PLATA – ARGENTINA)
	Experimental-theoretical approach applied to the study of Sr sorption in Na-Montmorillonite
P-22	ANDRÉS BIASETTI (CAB – ARGENTINA)
	Proposal for the characterization of a hydrogen storage system based on a hydride forming material using the neutrography technique

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