

1st TUMIEE Training School

“Training young researchers on multidisciplinary approaches to electronic excitation problems”

September 23 – October 4, 2019



Important dates:

June 30, 2019	Application deadline
July 15, 2019	Notification of acceptance
Sep 23 – Oct 4, 2019	Training School

Contact: ca17126@industriales.upm.es

More info: www.cost-ca17126.industriales.upm.es/activities/training-schools/

PURPOSE OF THE TRAINING SCHOOL

The goal of this training school is to disseminate the state-of-the-art in the field of electronic excitation, with special focus on young researchers, preferably PhD students already involved in research activities in the field. This will be framed within a multidisciplinary approach to electronic excitation, resulting in a general overview of the various simulation and experimental methods and techniques presently in use, and the areas that are in need of further advances. Progress along these lines will require an effort to *couple methods specifically developed to provide solutions within a restricted scope* (typically a specific time scale), in order to obtain more general quantitative results for the large variety of problems stemming from an initial electronic excitation of matter. This is the main goal of the Action, which will undoubtedly benefit from the work of young researchers in the coming years. In this sense, the Action through this school aims at sharing with the participants the necessary tools to go a step forward in their research. In addition, the School will foster the forging of new collaborative partnerships between participants.

With these ideas in mind, the 10-day school will be organized by means of general lectures in the mornings, and hands-on computer practical tutorials after lunch. For the tutorials, access to the supercomputer CESVIMA-Magerit will be granted. The general lectures are intended to provide an introduction to the tutorials and, more importantly, to provide a general description of the electronic excitation field to all the participants. For the tutorials, participants will be split in two groups, based on their major interests. The first group will concentrate on methods to study the effects of electronic excitation in short time scales, typically DFT, quantum kinetic methods, and molecular dynamics. The second group will concentrate on methods to obtain macroscopic responses, e.g., by means of post-irradiation analysis of experiments, Monte Carlo methods, finite element methods or hydrodynamics. Several sessions, including tutorials, will be devoted to the coupling of different methods. Current efforts will be explained as well as routes to get further progress in the coming years. The major outcome of the Action is expected to be a number of strategies to couple multidisciplinary methods and their application to cases of interest. We aim at sharing this progress and training a new generation of researchers by means of a second Training School to be held towards the end of the Action.

LIST OF TRAINERS

Tzveta Apostolova (BG)
Ana Benítez (ES)
Óscar Cubo (ES)
Fabiana da Pieve (BE)
Pablo de Vera (DE)
Vasilis Dimitriou (EL)
Flyura Djurabekova (FI)
Dorothy Duffy (UK)
Ioannis Ftilis (EL)
Mario García-Lechuga (FR)
Evangelos Kaselouris (EL)
Jorge Kohanoff (UK)
Vladimir Lipp (DE)

Layla Martin-Samos (IT)
Nikita Medvedev (CZ)
Alejandro Molina (ES)
Samuel Murphy (UK)
Eduardo Oliva (ES)
Gareth Owens (EL)
Nektarios Papadogiannis (EL)
Ovidio Peña (ES)
Antonio Rivera (ES)
Davide Sangalli (IT)
Andrey Solov'yov (DE)
Michael Tatarakis (EL)
Alexey Verkhovtsev (DE)

First week							
	Monday, Sep. 23 (House of Culture)		Tuesday, Sep. 24 (House of Culture)	Wed., Sep. 25 (House of Culture)	Thursday, Sep. 26 (House of Culture)	Friday, Sep. 27 (House of Culture)	Saturday, Sep. 28
9.00 – 10.50	Introduction: Electronic excitation - COST Action CA17126		Experimental methods: irradiation and characterization	In situ optical characterization	Time-resolved experimental techniques	Molecular dynamics, Langevin dynamics	
	Rivera, Benítez		Rivera, Peña	Peña	García-Lechuga	Murphy	
11.10 – 13.00	Overview on Radiation-Matter interaction and methodologies from fs to mesoscopic scale		DFT: basic concepts and linear response	TD-DFT and NEGF: from coherent real time propagation to scattering and quantum kinetics	Quantum kinetic formalisms	Minoan Civilization	Guided visit to Archeological site of Eleuftherna
			Kohanoff, Sangalli		Apostolova	Owens	
	Djurabekova			Kohanoff, Sangalli			Owens
Lunch (13.00 – 14.30)							
Tutorial Session 1: short time scales	Introduction to super-computing. Access to Magerit. Cubo	Quantum Espresso & Yambo	Ground state and absorption with Quantum Espresso and Yambo	Ab-initio Real time simulations in presence of laser pulses with Yambo	Hands on Quebec: quantum electronics Boltzmann equation code	Molecular dynamics	
14.30 – 18.00 (aprox.)*		Molina, Martín-Samos	Kohanoff, Sangalli, Martín-Samos, Molina	Molina, Sangalli, Martín-Samos	Apostolova	Murphy	
Tutorial Session 2: macroscopic		Binary collision code SRIM	Analysis of irradiation results: script development	Analysis of in situ irradiation experimental data: Track formation	Time-resolved experimental techniques	Time-resolved experimental techniques	
14.30-18.00 (aprox.)*		Rivera, Djurabekova	Rivera, Peña	Rivera, Peña	García-Lechuga	García-Lechuga	

(*) Tutorial Session 1 and Tutorial Session 2 will be held simultaneously. Trainees will be divided into 2 groups in most of these afternoon sessions as it is shown on the table (there are common sessions on the 23/09, 02/10 and 03/10). The sessions are expected to finish around 18.00 (aprox.).

Second week						
	Monday, Sep. 30 (House of Culture)	Tuesday, Oct. 1 (House of Culture)	Wed., Oct. 2 (House of Culture)	Thursday, Oct. 3 (Institute for Plasma Physics and Lasers)	Friday, Oct. 4 (Institute for Plasma Physics and Lasers)	Saturday, Oct. 5
9.00 – 10.50	Radiation hydrodynamics Oliva	FEM and MHD Numerical Simulations on Radiation-Matter Interactions Dimitriou	Monte Carlo methods II Da Pieve	Welcome on IPPL High Power Laser – Plasma Physics Tatarakis Ultrafast Lasers and high electronic excitation Papadogiannis	Visit the IPPL Laboratories Papadogiannis, Tatarakis, Ftilis	
11.10 – 13.00	Molecular dynamics, two-temperature models Duffy	Monte Carlo methods Medvedev	Coupling of methods (timescales) / experimental validation and applications Solov'yov	Coupling of methods (timescales) / experimental validation and applications II Solov'yov	Open discussion Summary and closing Tatarakis, Papadogiannis	
Lunch (13.00 – 14.30)						
Tutorial 1: short time scales 14.30 – 18.00 (aprox.)	Molecular dynamics Duffy	Monte Carlo Lipp	Code coupling; MBN software De Vera, Verkhovtsev	Code coupling; MBN software De Vera, Verkhovtsev		
Tutorial 2: macroscopic 14.30 – 18.00 (aprox.)	Radiation hydrodynamics Oliva	Laser matter interactions-Hands on FEM and MHD simulations Dimitriou, Kaselouris				

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