Towards understanding and modelling intense electronic excitation

First General Meeting (CA17126)
19th & 20th November 2018
Madrid, Spain

AGENDA

Monday, 19th November 2018	
8:00 - 9:00	Registration
9:00 - 9:30	Opening session
9:30 - 10:50	Session I: Introduction • 9:30 E. Oliva ⇒ Multiscale in plasmas: short pulses, ionization, collisional processes and hydrodynamics. • 9:50 S. Fahy ⇒ Electronic excitation – an overview of methods, models and time-scales. • 10:10 F. Djurabekova ⇒ Simulation of Elongation of Metal Nanoparticles by Swift Heavy Ions by the coupling of two-temperature models and molecular dynamics methods. • 10:30 A. Rivera ⇒ Overview of our Action CA17126 around an example, the absorption of fs-laser pulses by surface plasmons in nanoparticles.
10:50 - 11:10	Coffee break
11:10 - 13:10	Session II: Cases of interest ⇒ Presentations (13) + discussion
13:10 - 14:30	Lunch
14:30 - 16:10	Session III: Cases of interest ⇒ Presentations (11) + discussion
16:10 - 16:30	Coffee break
16:30 - 18:00	Workgroup meetings
20:00	Dinner at the restaurant “Mesón del Cid”

Tuesday, 20th November 2018	
9:00 - 10:50	Session IV: Cases of interest ⇒ Presentations (11) + discussion
10:50 - 11:10	Coffee break
11:10 - 12:10	Session V: WG vision ⇒ Summary of WG discussions (by WG Leaders)
12:10 - 13:10	Session VI: Accessible facilities and codes • 12:10 D. Sangalli ⇒ Overview of a few first-principles codes: what exists and what is needed to go towards the high-intensity multi-scale regime. • 12:25 A. Solov'yov ⇒ Multiscale modelling of complex molecular systems for modern technologies with MBN Explorer • 12:40 M. Flores ⇒ Laser Laboratory for Acceleration and other application at the USC: bio-applications. • 12:50 L. Volpe ⇒ Laser -Driven Particle Beams and Applications at CLPU. • 13:00 F. Sordo ⇒ Proposal for the use of ESS-Bilbao Proton Beam for high electronic excitation inside the CA17126.
13:10 - 14:30	Lunch
14:30 - 16:00	Session VII: Technical discussions • 14:30 ⇒ Selection of cases based on available methods and networking capabilities • 15:55 ⇒ Closing
16:00 - 16:20	Coffee break
16:20 - 18:00	2nd MC Meeting (only for MC Members)

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CASES OF INTEREST

SESSION I

I.1 **Multiscale in plasmas: short pulses, ionization, collisional processes and hydrodynamics**
Eduardo Oliva
Universidad Politécnica de Madrid, Spain

I.2 **Electronic excitation – an overview of methods, models and time-scales**
Stephen Fahy
University College Cork, Ireland

I.3 **Simulation of Elongation of Metal Nanoparticles by Swift Heavy Ions by the coupling of two-temperature models and molecular dynamics methods**
F. Djurabekova
University of Helsinki, Finland

I.4 **Absorption of fs-laser pulses by surface plasmons in nanoparticles**
Antonio Rivera
Universidad Politécnica de Madrid, Spain

SESSION II

II.1 **Non-linear wavefront distortion in high power laser optics**
Klaus Mann
Laser-Laboratorium Göttingen, Germany

II.2 **Solids under intense electronic excitation**
Nikita Medvedev
Institute of Physics and Institute of Plasma Physics, Academy of Science of Czech Republic

II.3 **Short- and long-timescale spatially-resolved distribution of energy absorbed in bulk materials after their X-ray irradiation**
Vladimir Lipp
CFEL, DESY, Germany

II.4 **Non-Thermal melting vs Thermal melting**
Layla Martin-Samos
CNR-IOM Democritos, Italia

II.5 **Ultrafast decay of low-symmetry photo-induced atomic forces**
Shane O'Mahony
Tyndall National Institute, Ireland

II.6 **Electron-phonon coupling at the surface of the topological insulator, Bi2Te3**
José Daniel Querales
University College Cork, Ireland

II.7 **Manifestations of high-dense particle excitation/irradiation in the spectra of wide-gap materials**
Aleksandr Lushchik
University of Tartu, Estonia

II.8 **Extreme states of matter with table-top radiation sources**
Karol Adam Janulewicz
Military University of Technology, Poland

II.9 **Electron plasmas as an instrument for exciting atomic nuclei**
Stoyan Mishev
New Bulgarian University, Bulgaria

II.10 **Theoretical modeling of ultrafast x-ray spectroscopy in molecular and condensed-matter systems**
Antonio Picón
Universidad Autónoma de Madrid, Spain

II.11 **Role of the ionization in supercontinuum generation in bulk and multi-plate media**
Julio San Román
Universidad de Salamanca, Spain

II.12 **Ultrafast x-ray vortex beams for studying spin-orbit interaction at the nanoscale**
Carlos Hernández-García
Universidad de Salamanca, Spain

II.13 **Non-linear response of solids to strong electromagnetic fields**
Luis Plaja
Universidad de Salamanca, Spain

SESSION III

III.1 **Computational studies of collision-induced processes with complex molecular systems**
Alexey Verkhovtsev
MBN Research Center at FiZ, Germany

III.2 **Modeling of inelastic collision processes in the course of propagation of charged particles in media**
Andrey V. Solov'yov
MBN Research Center at FiZ, Germany

III.3 **Highly efficient multiscale modelling of advanced materials: from an accurate description of electronic excitations to massively parallelised atomistic simulations**
Roberto Iglesias
Universidad de Oviedo, Spain

III.4 **Space Radiation effects at candidate landing sites for the ExoMars 2020 ESA mission: a Monte Carlo particle transport study**
Fabiana Da Pieve
Royal Belgian Institute for Space Aeronomy, BIRA-IASB, Belgium

III.5 **The role of the initial energy deposition during SHI irradiation**
Henrique Vázquez
University of Helsinki, Finland

III.6 **Temporal evolution of the electron distribution function (EDF) and atomic states in the presence of a short pulse (< 100 fs) high intensity x-ray laser radiation**
Pedro Velarde
Universidad Politécnica de Madrid, Spain

III.7 **Radiation chemistry resulting from electronic excitations**
Pablo De Vera
German Cancer Research Center, Germany

III.8 **Electronic excitation strategy in liver transplantation from cadaveric donors**
Carmen Peralta
Hospital Clinic de Barcelona, Spain

III.9 **Relevance of detection of liver steatosis**
Mª Eugenia Cornide-Petronio
Hospital Clinic de Barcelona, Spain

III.10 Optical Excitations in 2D Materials
Alejandro Molina-Sánchez
University of Valencia, Spain

III.11 Single-cycle CEP-stable intense light sources for field-dependent excitation and time-resolved electronic dynamics
Helder Crespo
Universidade do Porto, Portugal

SESSION IV

IV.1 Non-equilibrium Green's functions approach to radiation-induced electron dynamics in biological molecules
Enrico Perfetto
CNR-ISM, Italy

IV.2 Light-controlled currents in solids
István Magashegyi
University of Szeged and ELI-ALPS, Hungary

IV.3 Thermodynamic model of electron emission, negative and positive ion formation in keV molecular collisions
Zoltán Juhász
MTA Atomki, Hungary

IV.4 Ion-induced collision processes and subsequent chemical effects in polymers and their gas-phase monomers: an experimental multi-scale approach
Sándor Demes
MTA Atomki, Hungary

IV.5 Excitation and ionization of biomolecules by ion impact
Luis Méndez
Universidad Autónoma de Madrid, Spain

IV.6 Stress relief of thin film coatings with pulsed fluxes of highly energetic ions
Iván Fernández
Nano4Energy, Spain

IV.7 Electronic excitation and spectroscopy of laser-produced plasmas
Klaus Mann
Laser-Laboratorium Göttingen, Germany

IV.8 Interaction of intense nanosecond pulses of extreme ultraviolet (EUV) with matter
Andrzej Bartnik
Military University of Technology, Poland

IV.9 High harmonics from noble gas clusters: An evidence for nanoplasmas
István B. Földes
Wigner Research Centre for Physics of the HAS, Hungary

IV.10 Progress in modeling of non-equilibrium plasmas intensively radiating in EUV and soft X-ray range
Sergey V. Zakharov
Gamma Pulse, Palaiseau and EATS, France
NRC «Kurchatov Institute», Russia

IV.11 Dosimetry in irradiated water (to be confirmed)
Jorge Kohanoff
Queen's University Belfast, United Kingdom