

Panel “Filming Electrons in Motion”,

Thursday 3 September 2020 from 12:00 to 13:30 Room 27A

Abstract:

LEAPS - the League of European Accelerator-based Photon Sources - is a strategic consortium of Synchrotron Radiation and Free Electron Laser (FEL) user facilities. Over the last decades, high-flux and high repetition-rate accelerator-based photon sources have revolutionized a myriad of fundamental, applied and industrial sciences: the absolutely impressive and never-ending improvements of brightness, spectral range and degree of spatial and temporal coherence and resolution of the sources have deepened the understanding of electronic and structural properties of matter through element specific, chemical and spin selective probes. As a consequence, materials characterization has been developing towards increasing complexity regarding dimensionality, concentration and extreme or ambient environments. Combining femtosecond X-ray pulses with coherence and enormous peak brightness FELs have now enabled studies of a broad class of dynamic phenomena in matter that crosses many scientific disciplines and have led to major breakthroughs in the last few years. The ability of FELs to follow the steps of a chemical cycle or reaction like in a slow-motion movie will help to better understand natural or technical chemical processes, and push the development of original experimental strategies to study non-equilibrium behavior of matter at the femtosecond-nanometer time-length scales.

The session we propose will focus on the contribution of accelerator-based photon sources on three important subjects: (i) the new regime of X-ray matter interactions with ultrashort very intense X-ray pulses, (ii) the new potential of coherent imaging and scattering for answering questions about nano dynamics in complex materials and (iii) the unique possibility to stimulate and probe nonlinear phenomena that are at the heart of conversion of light into other forms of energy, relevant to photovoltaics, fs magnetism and phase transitions in correlated materials.

Majed Chergui, Professeur ordinaire, Laboratoire de spectroscopie ultrarapide EPFL - speaker, in person
Caterina Biscari, Director Alba Synchrotron - speaker, remote

Jan Lüning, Scientific Management Helmholtz-Zentrum Berlin für Materialien und Energie - speaker, remote

Stefan Eisebitt, Director at the Max-Born-Institut - speaker, remote

Claudio Masciovecchio, Director of the Focus Project Elettra - Sincrotrone Trieste - moderator, in person

Alfonso Franciosi, President and Chief Executive Officer Elettra - Sincrotrone Trieste - convenor, in person
or **Giorgio Paolucci**, Chief Scientific Officer Elettra - Sincrotrone Trieste - convenor, in person

Panel Project EXSCALATE4CoV (E4C) "The Exscalate4CoV project: a journey from HPC to virtual reality. How Computer-Aided Drug Design techniques are supporting the fight against SARS-CoV-2", Thursday 3 September from 18:45 to 19:30 Room 28H

Abstract:

The EXSCALATE4CoV (E4C) project is a collaboration between 18 EU organizations to fight against SARS-CoV-2 with advanced Computer-Aided Drug Design (CADD) methods and to accelerate the identification of drugs for future pandemics. At the core of the project is the exploitation of the EXSCALATE platform to identify the most promising safe in man drugs and de novo small molecules to be active against coronavirus.

In the early stages of the pandemic, no experimental structures existed for SARS-CoV-2 proteins and we bridged the gap by using SWISS-MODEL to generate predicted three-dimensional models. These models were later supplemented with experimental structures and used to run MD simulations on European HPC systems. The simulations were performed to virtual screen, the Safe in Man (SIM) library, containing the commercialized and developing drugs (> 10000), to identify the most promising safe in man drugs ready for immediate treatment of the infected population, and, in a second phase, the larger Tangible Chemical Space (TCS) library to identify new potential pan coronavirus inhibitors. With Nanome's virtual reality platform we can explore and analyze the results of the simulations collaboratively amongst the members of the consortium which are located in different geographic locations across Europe.

Gerardo Tauriello, Team Lead Software Development, Computational Structural Biology, Swiss Institute of Bioinformatics, speaker, remote

Edgardo Leija, Chief Experience Officer & Co-founder, Nanome Inc., speaker, remote

James Beacham, Chelonia Applied Science - Communications Ambassador, CERN, moderator, remote