European XFEL Theory Seminar

Thursday 15th June 2017, 17:00
Campus Schenefeld, main building (XHQ) room E1.172

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Predicting the unavoidable: simulations of high intensity X-ray induced dynamics of matter

A unique capability of the X-ray Free-electron Lasers (XFEL) is to produce extreme high intensity radiation. Matter exposed to even a single XFEL pulse becomes highly excited and exhibits complex time evolution. Enormous energy absorption happening on the femtosecond timescales brings matter into highly excited states via non-equilibrium dynamics. The non-linear nature of the dynamics makes the interpretation of measured data non-straightforward. As such a scenario is rather general for all high-intensity experiments (e.g. imaging, spectroscopy, etc.), the support from theory and simulations is becoming increasingly important.

In this talk we overview our approach of simulating XFEL irradiated finite size objects (e.g. atom clusters) as well as bulk matter. We discuss modeling challenges and possibilities. We give insight into our simulation framework based on a Monte Carlo/Molecular Dynamics concept that leads to a microscopic description of the sample. The model gives a full description of the X-ray induced dynamics, allowing to access time resolved data on the electronic configuration of individual ions, on ions' positions and velocities as well as those of the free-electrons, on fluorescent emission, etc. We demonstrate the predictivity of the model through its comparison to experimental data. Finally, we discuss perspectives for future simulations in the context of possible applications for the European XFEL.

Reference: www.desy.de/~xraypac

Host: Evgeny Gorelov