



**25<sup>th</sup> May 2016 - 2:00 p.m.**  
CFEL-bldg. 99, seminar room IV

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## **Modeling x-ray irradiation of matter: finite systems to bulk samples**

With the advent of x-ray free electron lasers the generation of super bright x-ray pulses is now a reality. These x-ray pulses find a variety of applications, especially in exploring different regimes of photon matter interaction. While the x-ray irradiation of complex molecules and noble gas clusters is an area of interest for single particle imaging application [1], modeling the complex interaction of these photon packets with bulk samples is a challenge for an emerging community of warm dense matter research [2]. We try to investigate these complex interactions and the resulting sample dynamics by using a range of in-house developed computational tools. In my talk I would outline the challenges in modelling the long time evolution of the nanoplasma, formed by the irradiation of large clusters and/or bio-molecules and discuss our approaches to overcome them. The focus would be on a two-step MD-hydrodynamic approach, wherein the first non-equilibrium phase is simulated with the molecular dynamics tool, XMDYN [3–5], while the later phase of collisional expansion of the nanoplasma is simulated by computationally much cheaper hydrodynamics approach [6, 7]. I would also discuss about our kinetic approach with most probable configuration scheme, to simulate the hard x-ray irradiation of bulk samples [8].

[1] R. Neutze *et al.*, *Nature* **406**, 752 (2000).

[2] S.M. Vinko *et al.*, *Nature* **482**, 5962 (2012).

[3] Z. Jurek, B. Ziaja, and R. Santra, XMDYN rev. 2272 (CFEL, DESY, 2016).

[4] B. Murphy, T. Osipov, Z. Jurek, L. Fang *et al.*, *Nature Communications* **5**, 4281 (2014).

[5] T. Tachibana, Z. Jurek, H. Fukuzawa, K. Motomura *et al.*, *Scientific Reports* **5**, 10977 (2015).

[6] V. Saxena, Z. Jurek, B. Ziaja, R. Santra, *High Energy Density Physics* **15**, 93 (2015).

[7] V. Saxena and B. Ziaja, *Physics of Plasmas* **23**, 012710 (2016).

[8] B. Ziaja, V. Saxena, S.-K. Son *et al.*, Accepted in *Physical Review E* (2016).