

# Simulation of Liquid Jet Explosions and Shock Waves Induced by X-Ray Free-Electron Lasers

Leonie Chatzimagas<sup>1</sup> and Jochen S. Hub<sup>1</sup>

<sup>1</sup>*Department of Theoretical Physics, Saarland University, Saarbrücken, Germany*

X-ray free-electron lasers (XFELs) produce X-ray pulses with very high brilliance and short pulse duration. These properties enable structural investigations of nanocrystals or single biomolecules, and they allow resolving the dynamics of biomolecules down to the femtosecond timescale. To deliver the samples rapidly into the XFEL beam, liquid jets are used. The impact of the X-ray pulse leads to vaporization and explosion of the liquid jet, while the expanding gas launches shock wave trains traveling along the jet that can affect biomolecular crystals before they have been probed. Here, we used atomistic molecular dynamics simulations to reveal the structural dynamics of shock waves after an X-ray impact. Analysis of the density in the jet revealed shock waves that form close to the explosion center and travel along the jet. A trailing shock wave formed after the first shock wave, similar to the shock wave trains in experiments. Although using purely classical models in the simulations, the resulting explosion geometry and shock wave dynamics closely resemble experimental outcomes, and they highlight the importance of the jet surface in shock wave propagation and attenuation.