European XFEL Joint Theory Seminar



Thursday, 9 November 2023, 16:00

XHQ / E1.041

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"Simulations of FELs and Ice"

X-ray sources pushing the frontier of intense ultrashort pulses have enabled the creation and investigation of exotic states of matter on Earth that were previously unobtainable. By probing an atomic cluster or large molecular system with an intense pulse from an Xray free-electron laser (XFEL) a system can transition into a plasma-like state that transiently retains the structure of molecular matter. This is true for water and ice, systems which are routinely studied with X-rays to reveal their diverse structures and anomalous properties, as well as for their relevance for the structure determination of biological macromolecules and protein crystals. In this work, we employ a hybrid collisional-radiative/molecular-dynamics method to study how X-ray pulses interact with hexagonal ice. We find that ice transitions into a crystalline plasma where its initial structure is maintained up to tens of femtoseconds. The ultrafast melting process occurs anisotropically, where different geometric configurations of the structure melt on different femtosecond time scales. The transient state and anisotropic melting of crystals can be captured by femtosecond X-ray diffraction, and this could impact any study of a crystalline structure probed by an XFEL.

Host: Nils Brouwer

Zoom link:

https://xfel.zoom.us/j/98713445171?pwd=WjZKRjJ4N1RXemVYVExWOEILZ2Q2UT09

Meeting ID: 987 1344 5171 Passcode: 629176

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