



20th April 2022 - 2:00 p.m.

CFEL-bldg. 99, seminar room IV and

[Virtual meeting room in ZOOM](#) (ID: 895 1951 2902 / PW: 925239)

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Plasma environmental effects in the atomic structure for simulating XFEL-heated solid-density matter

High energy density (HED) matter exists extensively in the Universe and can be created with extreme conditions in laboratory facilities such as x-ray free-electron lasers (XFEL). To better incorporate the nonlocality and nonthermal features of the XFEL-created dense plasmas, a hybrid quantum-classical approach based on a Monte Carlo-molecular dynamics (MC-MD) scheme has been proposed and implemented in XMDYN.

The ionization potential depression (IPD) phenomenon induced by plasma screening is indispensable in accurate modeling of dense plasmas, but it has not been included in any MC-MD plasma simulations. In this talk, the formation dynamics of dense plasmas is simulated employing the hybrid approach with plasma environmental effects via a recently proposed transient nonequilibrium IPD approach is presented. The importance of the IPD effect is demonstrated in theoretical modeling of dense plasmas by comparing two results with and without the IPD effects in the atomic structures that are exploited in XMDYN plasma simulations. The equilibrium charge state result of the plasma simulation with IPD shows a good agreement with the full quantum mechanical average-atom model simulation based on thermal equilibrium.

Host: Robin Santra – CFEL-DESY Theory Division