Joint Theory Seminar European XFEL, CFEL & Prof. Lichtenstein's Group at University of Hamburg



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XHQ/E1.173, in hybrid mode

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Predictions of novel features in x-ray scattering spectra for thermometry

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Design and interpretation of inertial confinement fusion experiments rely on accurate models of material properties far from ambient temperatures and densities. Validation of these models with data from focused experiments is in turn limited by uncertainties in measured sample conditions. In particular, electronic temperatures in the warm dense matter regime are typically inferred from detailed balance of plasmon features in x-ray Thomson scattering spectra, but this approach loses sensitivity for thermal energies above the plasmon energy. Using real-time time-dependent density functional theory, we predict that spectral features arising from scattering into thermally depleted core orbitals can be used as alternative diagnostics at higher temperatures. Our firstprinciples calculations for aluminum and iron heated to 1 eV and 20 eV validate a simpler average-atom model modified to capture behavior near solid densities. Furthermore, we uncover subtle signatures of atomic order at comparable energy transfers, offering opportunities for simultaneous inference of ionic and electronic temperatures which may be out of equilibrium during e.g., laser heating. This work advances characterization techniques critical for understanding the performance of materials in extreme environments. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

Hosts: Nils Brouwer and Beata Ziaja-Motyka

Zoom link: https://xfel.zoom.us/j/93724379268?pwd=MnZFRVRvT0RQWkl3K2hoaGdNM3kwZz09

Meeting ID: 937 2437 9268 Passcode: 386490

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