European XFEL Joint Theory Seminar

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European XFEL, Auditorium / Lighthouse

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On some interesting developments in warm dense matter theory

Even though warm dense matter physics, high energy density physics, or high pressure physics has come a long way, many challenges remain [1,2,3]. In theory and modelling of such states, we grapple with xc functionals of unknown quality in density functional simulations or with the Fermion sign problem in exact path integral Monte Carlo calculations. In experiment, we struggle with measurements that are too dependent on theory support.

Here, we show recent attempts to quantify the merits of different xc functionals for high pressure hydrogen for the case of the insulator to metal transition from basic considerations [4]. We also show a method to obtain the static electronic structure factor from DFT to high precision, which is useful for XRD on hydrogen [5]. We also have some suggestions for the enhancement of efficiency in simulations and experiment in order to increase experimental throughput, data collection, and analysis [6,7].

[1] Bonitz et al., Toward first principles-based simulations of dense hydrogen, Phys. Plasmas 31, 110501 (2024).

[2] Dornheim et al., Electronic density response of warm dense matter, Phys. Plasmas 30, 032705 (2023).

[3] Vorberger et al., Roadmap for warm dense matter physics, arXiv:2505.02494, PPCF (2026).

[4] Vorberger et al., Van-der-Waals exchange-correlation functionals and their high pressure and warm dense matter applications, arXiv:2511.11061 (2026).

[5] Moldabekov et al., Ab initio density functional theory approach to warm dense hydrogen: From density response to electronic correlations, Matter Radiat. Extremes 11, 025401 (2026).

[6] Moldabekov et al., Enhancing the efficiency of time-dependent density functional theory calculations of dynamic response properties, arXiv:2510.01875 (2025).

[7] Gawne et al., Spectral deconvolution without the deconvolution: Extracting temperature from X-ray Thomson scattering spectra without the source-and-instrument function, arXiv:2510.26747 (2026).

Host: Ruslan Kurta

Virtual participation (via Zoom):
https://xfel.zoom.us/j/67195395332?pwd=9iCCRjxOGP5M9mao6hsCW0b2ibvgsj.1
Meeting ID: 671 9539 5332
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