Warm dense matter: what theory is telling experiment, what theory could tell experiment, and why method developers should care

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An increasingly common application of electronic structure theory is the parameterization of material models used in laboratory astrophysics, inertial confinement fusion, and planetary science. In the context of thermodynamic properties like equation-of-state, this is well-aligned with the interests of method developers who have been seeking to improve the accuracy of total energy calculations since time immemorial. However, other properties vital to these applications, like conductivities and stopping power, have received somewhat less attention as a target for development. The central thesis of my talk is that more method developers should take notice of exciting opportunities to test their theories and codes against observables beyond thermochemistry.

While I will generally focus on Sandia's use of real-time time-dependent density functional theory (TDDFT) to study some of these observables, I will pay particular attention to its application in describing X-Ray Thomson Scattering experiments. Here, different approaches to calculating the experimentally-probed dynamic structure factor can be in conflict, making it somewhat difficult to assess how well theory is doing and the extent to which we should use it to make experimental inferences. Throughout my talk, I also hope to provide pedagogical details concerning the implementation and use of TDDFT in a plane-wave code, with some hints as to directions we are taking to adapt our methods to the computationally-challenging warm dense regime.

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