

Real-time dynamics of warm dense matter

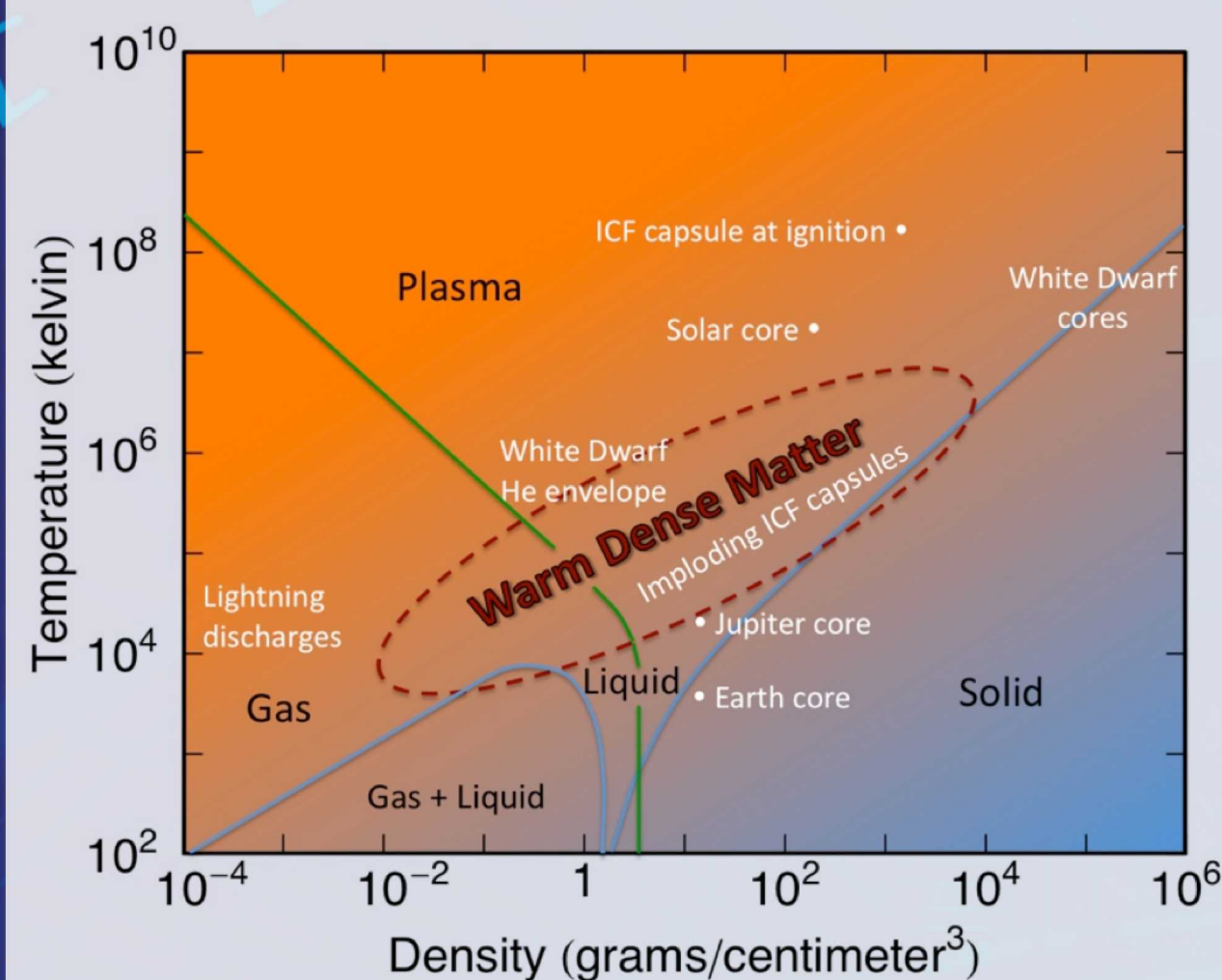
Sandia National Laboratories

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Problem

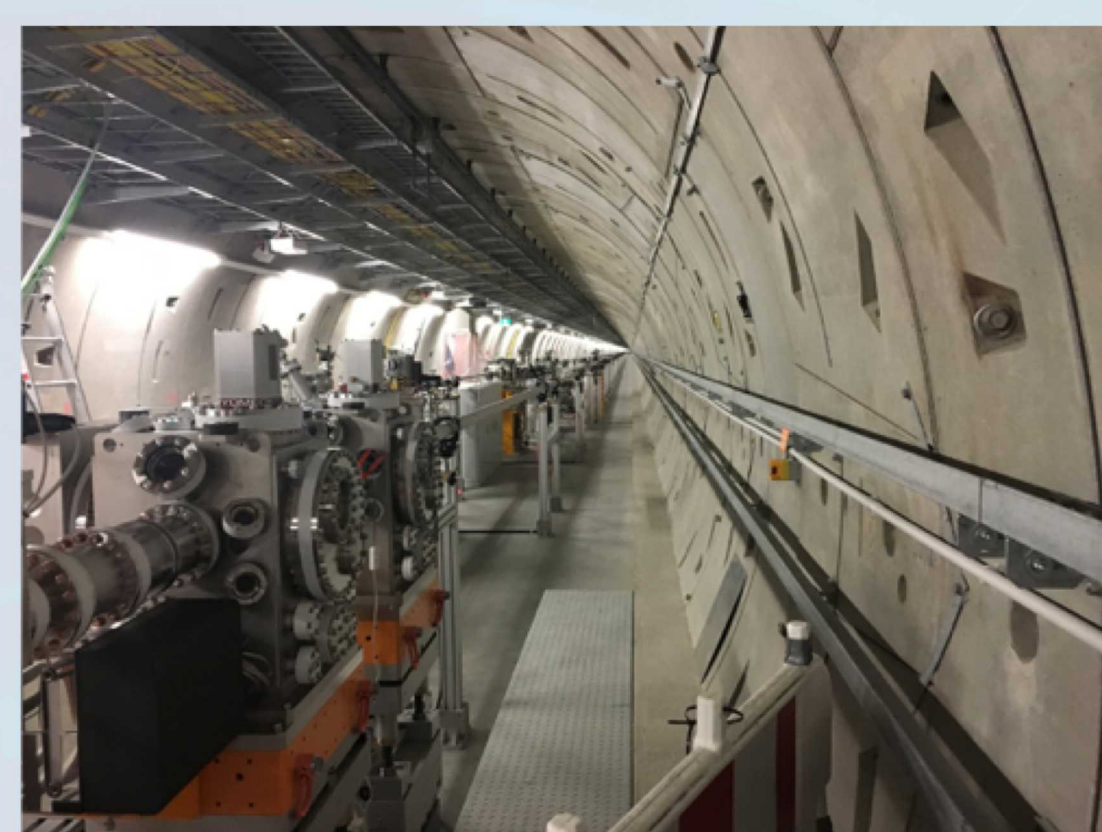


Warm dense matter:
neither solid nor plasma,
requires sophisticated
quantum simulation

Relevant to SNL mission
and fundamental physics

X-ray Free-Electron Lasers (XFELs) are a powerful tool for creating & probing warm dense matter

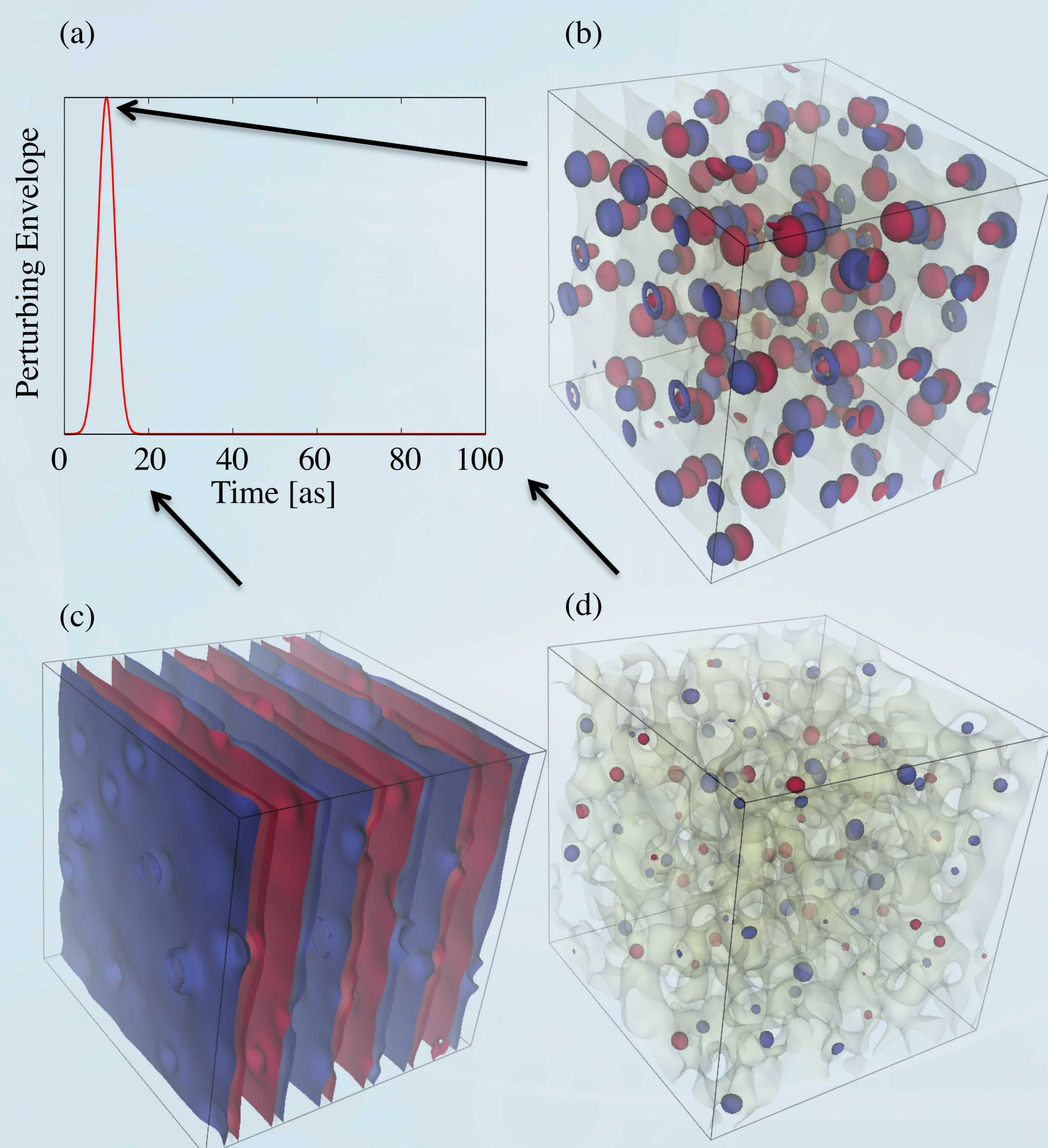
How can modeling and theory help to interpret experiments?



European XFEL (Hamburg)

Approach

First application of time-dependent density functional theory (TDDFT) to warm dense matter [Baczewski, et al., *Phys. Rev. Lett.*, 2016]

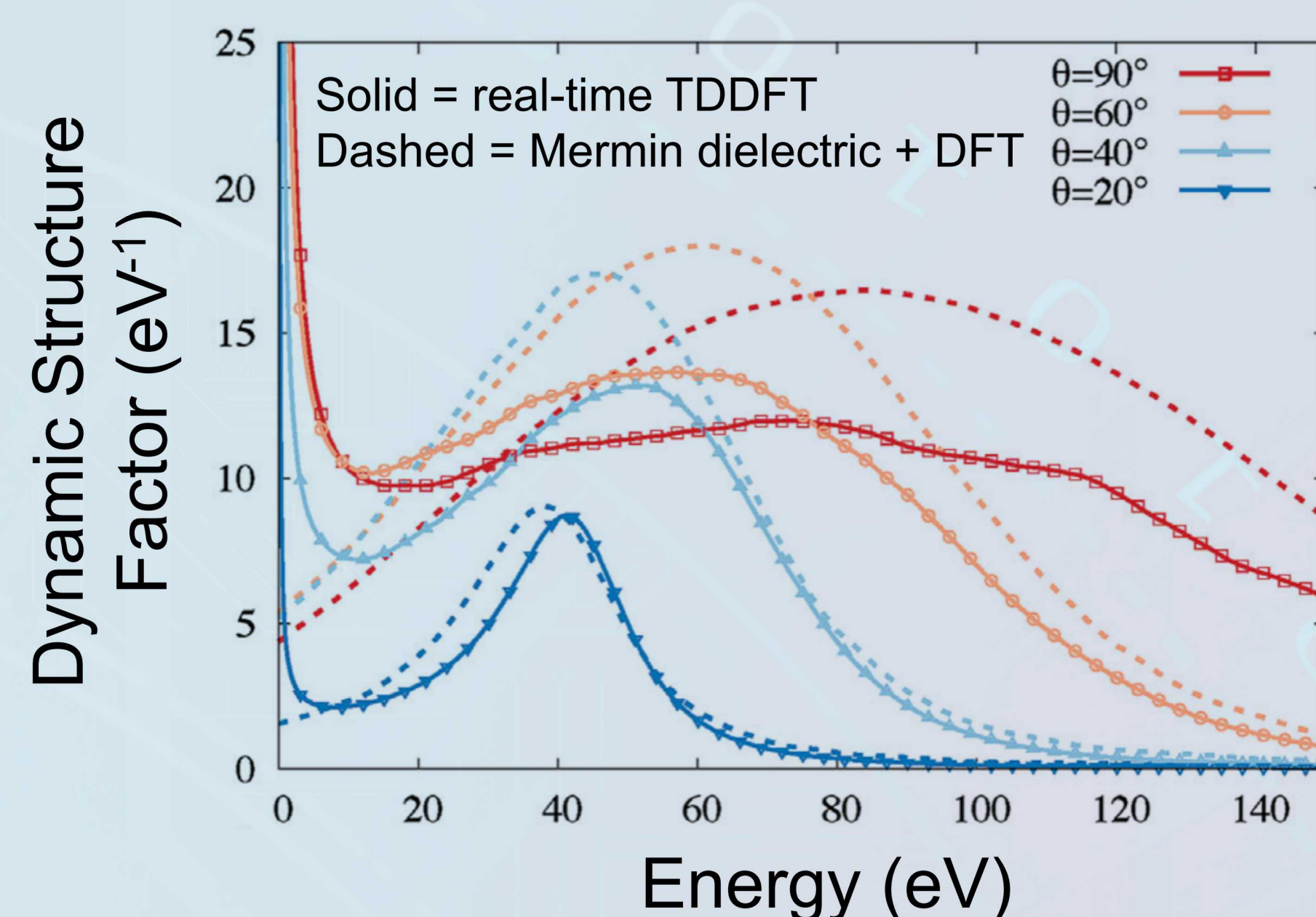


X-ray response of warm dense beryllium

Results

Theories with additional approximations are used to infer transport properties (DC conductivity)

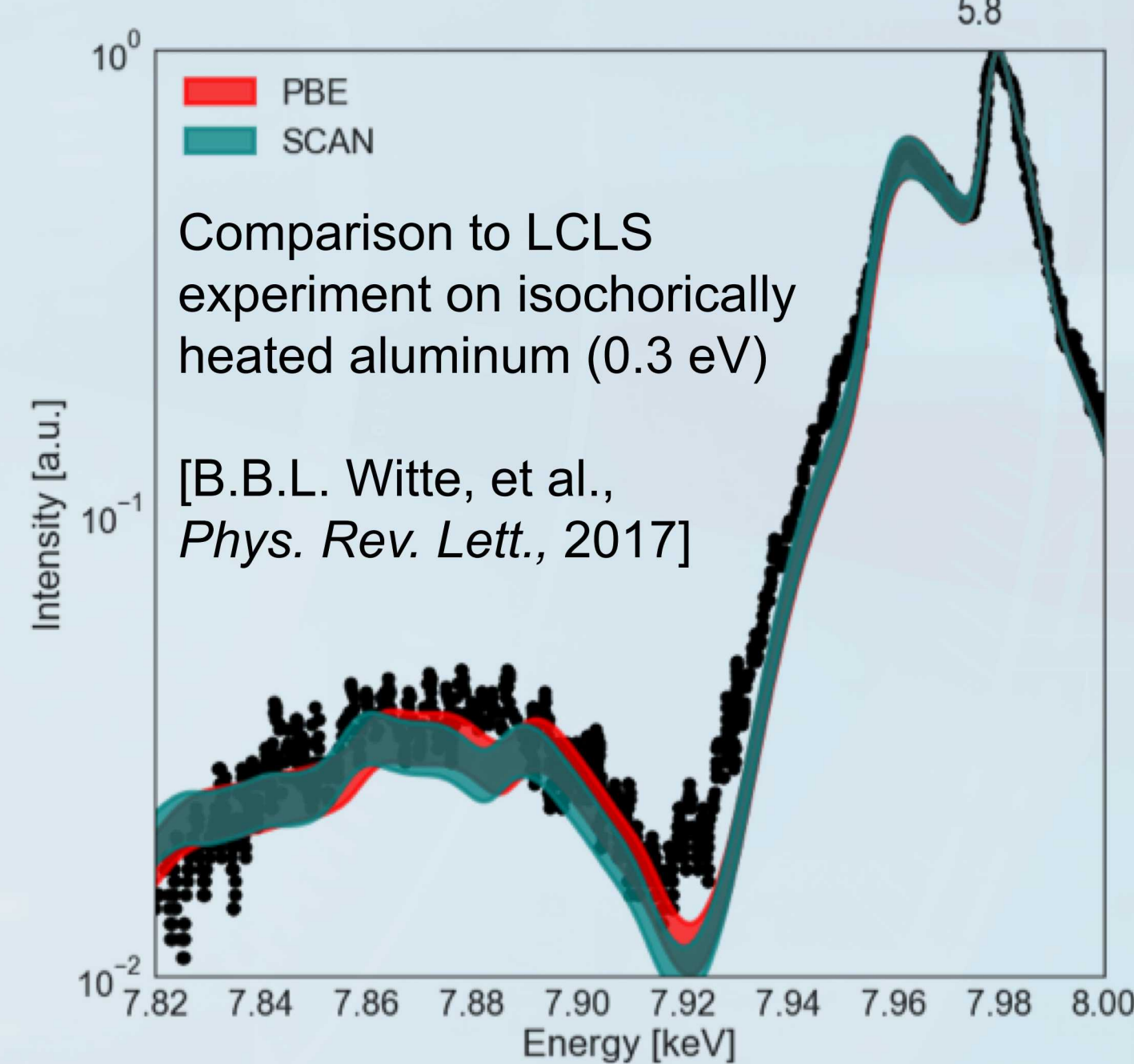
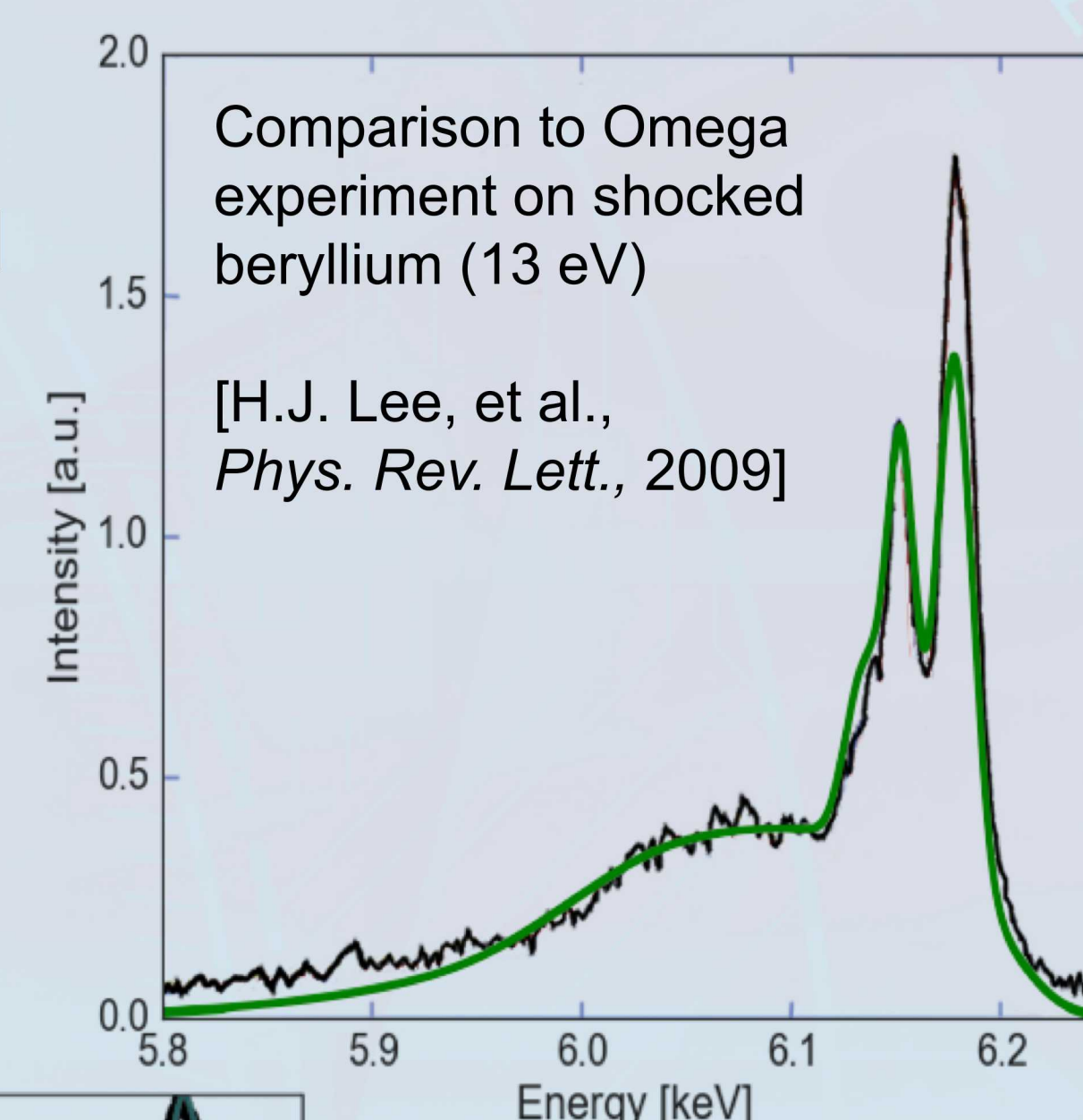
When is this valid?



Consistent at small scattering angles

At large scattering angles, we agree well with experiment

X-ray source brightness jumped 9 orders of magnitude in 2009 (LCLS)



Modeling support of XFEL experiments coming online now promise to help experimentalists infer new physics

Significance

Calculations on DOE HPC resources **explain and constrain experiments** at leading facilities like Z, NIF, Omega, and LCLS

One example of Sandia's expertise in all aspects of quantum simulation