Abstract Submitted
for the DPP19 Meeting of
The American Physical Society

Multiconfiguration Opacities from an Average Atom Model[1]
STEPHANIE HANSEN, Sandia National Laboratories — Average-Atom models based on density functional theory provide a self-consistent picture of electronic structure in high energy density plasmas, providing essential input for equation of state and conductivity tables. While opacities derived from average-atom wavefunctions (e.g. by Kubo-Greenwood) have the attractive feature of natively including dense plasma effects such as continuum lowering and pressure ionization, they lack both the accuracy in transition energies and the detailed structure necessary to calculate reliable opacities. Here we demonstrate a technique to efficiently generate detailed multiconfiguration atomic structure and spectra through a Taylor expansion of Slater coefficients. The basis wavefunction include both bound states and the "scars" of pressure-ionized bound states, ensuring smooth changes under density variations and extending self-consistent dense plasma effects from the average atom to a multiconfiguration model.

[1]Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA-0003525. This work was supported by the U.S. Department of Energy, Office of Science Early Career Research Program, Office of Fusion Energy Sciences under FWP-14-017426.

Stephanie Hansen
Sandia National Laboratories

Date submitted: 03 Jul 2019 Electronic form version 1.4