Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

The Korringa-Kohn-Rostoker Method Applied to Warm Dense Matter[1] DANIEL FINKENSTADT, U.S. Naval Academy, Physics Dept., Annapolis, MD, CHARLES E. NEWNAM, U.S. Naval Academy, Aerospace Dept., Annapolis, MD, BRIAN G. WILSON, Lawrence Livermore National Laboratory, Livermore, CA — The electronic structure, EOS and transport properties of warm electrons in an amorphous or disordered configuration of ions is not well described by either solid-state or plasma models. Such warm, dense systems share the characteristic of the solid state that multi-center scattering effects are of paramount importance in forming bands of valence states. Theoretical treatment of the EOS of warm, dense matter therefore requires a way to include significant occupation of higher energy and angular momentum channel continuum states. We are extending the Green's function Kohn-Korringa-Rostoker code *MECCA* as an all-electron (non-pseudo potential) method that treats arbitrary mixtures of atoms on an ab-initio basis over a broad range of conditions, from cold, solid matter up to hot plasmas at extreme (ICF) compression. Specific examples of Aluminum and Boron-Nitride will be discussed.

[1]Supported by the Military Academy Research Associates program, LLNL/USNA.

Daniel Finkenstadt
U.S. Naval Academy, Physics Dept., Annapolis, MD

Date submitted: 19 Dec 2011 Electronic form version 1.4