Equation of State of Hot Dense Li-D from Green's Function KKR electronic Structure

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The MECCA code is a green's function based KKR algorithm originally developed at the University of Illinois for the study of solid-state properties of complex crystals, alloys and materials with site defects. The ground state electronic structure is calculated in periodic unit cells of user specified mixtures of nuclei at fixed positions. We have recently generalized[1] this approach to calculate the average electronic structure and thermodynamic properties of *thermal* electrons as a means of extending beyond homonuclear average-ion-in-jellium plasma models for Equation of State.

We present results for a Li-D EOS table generated over a broad range of temperatures and densities, under a crude approximation of two atom unit cells using a cold NaCl crystal lattice structure, and compare with results generated from the LLNL PURGATORIO[2] plasma model. Prospects for more definitive calculations employing averages over ensembles of ion configurations (in larger super-cells with more nuclei per unit cell at randomized positions) will be discussed.

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[1] B. Wilson, D. Johnson, A. Alam, High Energy Density Physics 7 (2011) 61

[2] B. Wilson, V. Sonnad, P. Sterne, W. Isaacs, J.Quant. Spect. Radiat. Transfer 99 (2006) 658