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PIMC Validation of Effective Quantum Potentials for MD Simulations of Dense Plasmas HEATHER D. WHITLEY, JOHN I. CASTOR, A. BRUCE LANGDON, SAAD A. KHAIRALLAH, MICHAEL P. SURH, JONATHAN L. DUBOIS, BERNI J. ALDER, ERIK W. DRAEGER, ERIC SCHWEGLER, FRANK R. GRAZIANI, Lawrence Livermore National Laboratory, MICHAEL S. MURILLO, Los Alamos National Laboratory, CIMARRON COLLABORATION — Molecular dynamics (MD) simulations of dense plasmas, such as those found in non-equilibrium laser fusion experiments, are challenging due to the importance of several quantum mechanical effects. We currently employ approximate statistical potentials, obtained exactly in the pair approximation from a numerical solution of the Bloch equation for the Coulomb density matrix. The fermionic character of the electrons is handled via an effective Pauli potential. We first study the accuracy of existing pair potentials and their extension to lower temperature and high Z ions by examining the exact pair density matrix. We then perform classical hypernetted chain and MD simulations using those effective potentials to study equilibrium thermodynamics of dense plasmas. Fully quantum path integral Monte Carlo (PIMC) simulations are used to gauge the accuracy of the classical calculations for dense hydrogen. Using feedback from the PIMC, we can further refine the effective Coulomb and Pauli potentials. Prepared by LLNL under Contract DE-AC52-07NA27344.

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