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Quantum Molecular Dynamics calculation of electrical and thermal transport properties MICHAEL P. DESJARLAIS, Sandia National Laboratories — Dense, strongly-coupled plasmas, with degenerate or partially degenerate electrons — ubiquitous in high energy density physics, inertial fusion, planetary science, and warm dense matter — are very difficult to describe accurately with traditional theoretical approaches. Over the last decade, density functional based molecular dynamics, also know as quantum molecular dynamics (QMD), has emerged as a powerful tool for the study of dense quantum plasmas, providing accurate equation of state, structural, and transport properties. This talk will focus on the QMD calculation of electrical and thermal conductivities with a much higher degree of accuracy than was possible with earlier methods. Within the density functional approach, electrical and thermal conductivities are extracted directly from the electronic orbitals using the Kubo-Greenwood and Chester-Thellung formalisms, circumventing the need to define the ionization states and collision cross sections. These transport calculations have now been used to generate several wide-range transport models for use in large-scale simulation codes, allowing unprecedented simulations of complex experiments. Sandia National Laboratories is a multi program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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