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Thermoelectric transport properties of warm dense molybdenum from first-principles simulations MARTIN FRENCH, THOMAS HAILL, MICHAEL DESJARLAIS, THOMAS MATTSSON, Sandia National Laboratories — Molybdenum, with its high melting point, significant electrical conductivity, and high material strength, is a technologically important material in general and has in particular recently been proposed as a driver material in high-pressure strength experiments on Sandia's Z-machine [1]. To simulate and understand the processes in these experiments with magneto-hydrodynamic simulations, accurate models for the electrical and thermal conductivity are needed for a wide range of thermodynamic parameters. Here, we present novel results for the electrical and thermal conductivity of molybdenum in various states ranging from the solid to the dense plasma phase. The results were obtained with first-principles simulation techniques that combine density functional theory with molecular dynamics and linear response theory. We find good agreement between our theoretical results and available experimental data. Sandia National Laboratories is a multiprogram laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the US Department of Energy's National Nuclear Security Administration under Contract No. DE-AC04-94AL85000.

[1] C. S. Alexander, J. R. Asay, T. A. Haill, J. Appl. Phys. 108, 126101 (2010)

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