First-principles entropy calculations for liquid metals and warm dense matter MICHAEL DESJARLAIS, Sandia National Laboratories*, Albuquerque, New Mexico — The total entropy is not an explicit or easily accessible quantity in first-principles molecular dynamics simulations. It is, however, an extremely important quantity for the calculation of total free energies and derived properties such as equilibrium phase boundaries. In shock experiments the entropy of the shock state determines the release isentrope. Recent advances in the calculation of the entropy for liquid metals and warm dense matter directly from the velocity history in quantum molecular dynamics simulations are presented. The method, a generalization of the 2PT method for classical molecular dynamics [Lin, *et al.*, J. Chem. Phys. 2003], significantly increases the accuracy of the method for systems with electronic entropy, spin degrees of freedom, and the softer interactions characteristic of liquid metals and warm dense matter. The results are compared to data and the results of indirect methods, such as coexistence simulations to determine phase boundaries.

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