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Modeling of electron-ion coupling in shocked materials EVAN REED, Stanford University — This work describes and implements a quasi-statistical approach to electron-ion coupling in shocked matter. By combining this approach with the multi-scale shock technique (MSST) and a tight-binding model, the magnitude and role of electronic excitations in shocked energetic materials are studied theoretically using quantum molecular dynamics simulations. Focusing on the detonating primary explosive HN3 (hydrazoic acid), this work finds that the material transiently exhibits a high level of electronic excitation characterized by carrier densities in excess of 10^{21} cm^{-3}, or one electronic excitation for every 8 molecules. Electronic excitations enhance the kinetics of chemical decomposition by about 30%. The electronic heat capacity has a minor impact on the temperatures exhibited, on the order of 100 K.

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