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A semi-metallic layer in detonating nitromethane[1] EVAN REED, RIAD MANAA, LAURENCE FRIED, KURT GLAESEMANN, Lawrence Livermore National Laboratory, JOHN JOANNOPOULOS, Massachusetts Institute of Technology — We present the first ever glimpse behind a detonation front in a chemically reactive quantum molecular dynamics simulation (up to 0.2 ns) of the explosive nitromethane (CH_3NO_2) represented by the density-functional-based tight-binding method (DFTB). This simulation is enabled by our recently developed multi-scale shock wave molecular dynamics technique (MSST) that opens the door to longer duration simulations by several orders of magnitude. The electronic DOS around the Fermi energy initially increases as metastable material states are produced but then later *decreases*, perhaps unexpectedly. These changes indicate that the shock front is characterized by an increase in optical thickness followed by a reduction in optical thickness hundreds of picoseconds behind the front, explaining recent experimental observations. We find that a significant population of intermediate metastable molecules are charged and charged species play an important role in the density of states evolution and a possible Mott metal-insulator transition.

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