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Ab initio simulation of the Helium Hugoniot up to very high temperatures. GILLES ZERAH, STEPHANE LEROUX, CEA-DAM Ile de France — The advent of very high energy lasers will allow probing extreme states of matter, and in particular inducing extremely strong shocks. These new experiments begs for the development of techniques capable of addressing these extreme states of matter using first principle techniques in order to probe our current understanding of physics in these regimes. In this paper, we consider First Principles Molecular Dynamics simulations, which have already shown to be a very powerful tool for dense plasmas simulations. Up to now these simulations were limited to temperatures up to approximately 10eV as a consequence of the very rapid growth of the number of electronic states when solving the Mermin-Kohn-Sham effective Schrödinger equation. In this talk, we will present a new technique, based on a direct evaluation of the density matrix, which bypasses the need to compute eigenstates and therefore allow simulation up to very high temperatures (here, up to 100eV). We apply this method to the computation of the Hugoniot curve of cryogenic Helium, and compare our results with Path Integral Monte Carlo simulations and recent experimental data.

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