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Ab initio methods for modelling and simulation of warm dense hydrogen: how to get beyond Born-Oppenheimer approximation?

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Insulator-to-metal transition (IMT) in fluid warm dense hydrogen (WDH) is one of the unresolved problems of the last decades. There are a large number of experiments aimed at determining this transition, but they have a large number of disagreements among themselves.

Today, the theoretical description of experiments has come down to the use of *ab initio* methods. One of the most used is the Born-Oppenheimer dynamic with finite-temperature density functional theory (FT DFT). This method assumes that at each step the system has a certain average (fractional) distribution of electrons over states. Accordingly, it is important to understand that for this method to work, it is necessary that the electron transition times between these states are significantly less than the molecular dynamics step. To verify this assumption, it is necessary to move away from DFT and use methods in which the dynamics of electrons is considered explicitly.

The aim of this work is to study the IMT problem by non-adiabatic *ab initio* methods that would allow us to consider the non-equilibrium nature of this IMT that has not been considered previously in its theoretical assessments.

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