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Molecular dynamics simulation of temperature relaxation in dense hydrogen with electron force field method QIAN MA, JIAYU DAI, JING ZHAO, ZENGXIU ZHAO, National University of Defense Technology — Temperature relaxation between ion and electron is a pivotal non-equilibrium process. Molecular Dynamics (MD) is considered as the most effective method to deal with this problem. But the conventional classical MD regards not only ions but also electrons as charged points, which may lose some important physical process, such as ionization, rebound. To deal these problems we use the electron force field (eFF) method. The eFF method was firstly used by Julius T. Su and William A. Goddard III and it includes quantum effects as well as classical electrostatic interactions. It assumes that the electron is represented by a floating Gaussian wave packet and the whole wave packets are combined with Hartree product. The eFF method is found to be valid to describe the property of warm dense hydrogen. Here we want to use this method to investigate the electron-ion temperature relaxation process which includes the excited electrons and bound electrons. At the same time, the Coulomb Catastrophe in classical molecular dynamics may be avoided.

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