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Complex transport properties of warm dense Hydrogen: inclusion of nuclear quantum effects JIANMIN YUAN, DONGDONG KANG, JIAYU DAI, HUAYANG SUN, ZENGXIU ZHAO, National University of Defense Technology — Scattering or Collisions are the key physics in determining the transport properties for electrons and ions. Here we show based on ab initio (path-integral) molecular dynamics simulations, by including the Nuclear quantum effects (NQEs), the transport properties of warm dense hydrogen up to 1 eV can be significantly different from the results without NQEs. With the inclusion of NQEs, ionic diffusions are strongly enhanced by the magnitude from 100% to 15% with increasing temperature, while electrical and thermal conductivities are significantly suppressed. In particular at the temperature of 1 eV, where the NQEs have little effects on the static structures, the diffusion is still much larger than that without NQEs. The significant quantum delocalization of ions introduces expressively different scattering cross section between protons compared with classical particle treatments, which can explain the large alterability of transport behaviors. Furthermore, the Stokes-Einstein relation, energy, pressure, and isotope effects are also greatly influenced by NQEs. The complex behavior shows that NQEs cannot be neglected for dense hydrogen even in the warm dense regime. (arXiv:1304.0953 (2013))

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