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Nuclear quantum dynamics in warm dense hydrogen JIANMIN YUAN, DONGDONG KANG, JIAYU DAI, HUAYANG SUN, National University of Defense Technology — Quantum dynamics is a challenging problem in atomic and molecular dynamics. Ionic and electronic transport behaviors are strongly dependent on their dynamics, whose key physics is the scattering or collisions between particles. We usually consider only the quantum effects of electrons, but neglect the quantum effects of ions. Here, we show that the nuclear quantum effects can induce quantum tunneling in warm dense hydrogen, resulting in larger ionic diffusions and less electronic transport such as electrical and thermal conductivities. In order to study the nuclear quantum dynamics, we modify the sampling formula in path integral molecular dynamics (centriod molecular dynamics, CMD). Using the new sampling, the tunneling probability from CMD is consistent with the results of WKB approximation and full quantum mechanical calculations near the classical limit. 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. The complex behavior shows that NQEs cannot be neglected for dense hydrogen even in the warm dense regime, which would be important for the giant planets and inertial confinement fusion.

Zengxiu Zhao
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