Abstract Submitted
for the DPP16 Meeting of
The American Physical Society

Quantum simulation of structure, transport properties, and melting in dense hydrogen DONGDONG KANG, JIAYU DAI, JIANMIN YUAN, National University of Defense Technology — Due to the low mass, hydrogen exhibits significant nuclear quantum effects (NQEs), especially under low temperatures and high pressures. NQEs on structure and transport properties of dense liquid hydrogen under extreme conditions are investigated using the improved centroid path integral molecular dynamics (PIMD) simulations. The results show that with the inclusion of NQEs, the radial distribution functions are obviously broadened. The self-diffusion is largely higher while the shear viscosity is notably lower than the results of without the inclusion of NQEs due to the lower collision cross sections even when the NQEs have little effects on the static structures. The electrical conductivity is also significantly affected by NQEs. Quantum nuclear character induces complex behaviors for ionic transport properties of dense liquid hydrogen. In addition, the melting temperature of dense hydrogen is also investigated using the two-phase approach based on the PIMD with the Yukawa potential describing the interaction between ions. The results show that the NQEs have a significant impact on the melting of dense hydrogen, which largely lower the melting temperature by ~10% at the density range of 10-1000 g/cm^3.

Zengxiu Zhao
National University of Defense Technology

Date submitted: 17 Aug 2016 Electronic form version 1.4