DYNAMICAL PROPERTIES OF WARM DENSE HYDROGEN

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Dynamic properties of hydrogen fluid at high pressures and temperatures, which are difficult to access experimentally, are of particular interest to the scientific community. In 2020, the authors [1] used a machine-learned interatomic potential demonstrated the possibility of calculating the diffusion coefficient in warm dense hydrogen fluid. Subsequently, in work [2] within the framework of electronic density functional theory, taking into account isotopic effects for H_2/D_2, it was shown that near the fluid-fluid phase transition region, a significant increase in particle mobility is observed. Both mentioned works indicate an anomalous increase in diffusion, but the causes of this phenomenon are not yet fully understood. In the present study [3], we propose an explanation for this anomalous increase in particle mobility. Classical molecular dynamics with a machine-learned DeepMD interatomic potential, developed based on quantum mechanical calculations in the VASP package, is used to predict diffusion coefficients and shear viscosity (Fig. 1). The dependencies of the vibration spectrum, as well as diffusion coefficients and shear viscosity, on hydrogen density along isotherms in the temperature range of 600–1100 K are studied.

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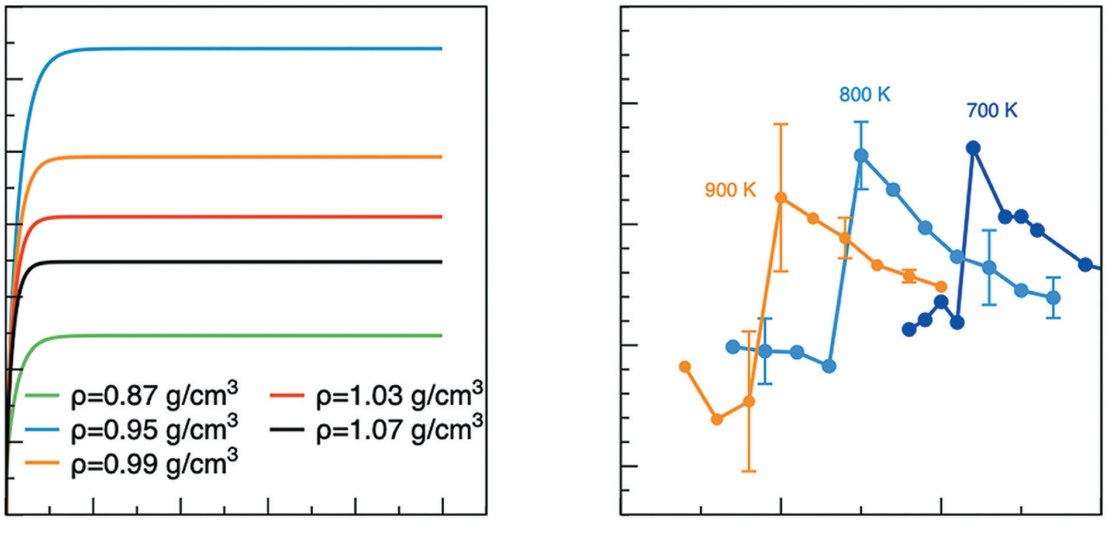

Fig. 1. The Green-Kubo integrals convergence for the different densities at 800 K (left) and the shear viscosity dependencies on density at various temperatures (right). The viscosity coefficients increase sharply at the same densities, as diffusivities, also indicating the occurrence of phase transition at these conditions

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