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Self-diffusion and viscosity for warm dense systems by orbital-free density functional theory TRAVIS SJOSTROM, JEROME DALIGAULT, Los Alamos National Laboratory — Evaluation of transport properties requires significantly longer molecular dynamics simulations than, for example, equation of state calculations. The standard approach at lower temperatures is to use Kohn-Sham (orbital dependent) density functional theory to find the quantum electron density at every molecular dynamics step. However, the Kohn-Sham approach becomes computationally prohibited at higher temperatures for equation of state, let alone for transport properties. Our recent orbital-free approach [Phys. Rev. Lett . 113, 155006] has shown excellent agreement with Kohn-Sham method at lower temperatures and extends to very high temperatures . Here we evaluate self-diffusion and viscosity from low to high temperatures and compare with Kohn-Sham methods where applicable as well as with recent approaches of kinetic theory.

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