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Diffusion time-scale invariance, randomization processes, and memory effects in Lennard-Jones liquids

Yulmetyev R., Mokshin A., Hänggi P.
Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

An approach for calculating transport properties based on the realization of idea of time-scale invariance of relaxation processes in liquids by Zwanzig-Mori memory function formalism was discussed. The approach was tested on Lennard-Jones (LJ) liquids. The diffusion coefficients of LJ liquids were calculated for a wide range of densities and temperatures. The results obtained were compared with the predictions of other theories and the molecular dynamics data.