



A molecular dynamics investigation of dynamical heterogeneity in supercooled water

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We investigate the presence of dynamical heterogeneity in supercooled water with molecular dynamics simulations using the new water model proposed by Mahoney and Jorgensen [M.W. Mahoney, W.L. Jorgensen J. Chem. Phys. 112, 8910 (2000)]. Prompted by recent theoretical results [J.P. Garrahan, D. Chandler, Phys. Rev. Lett. 89, 35704 (2002)] we study the dynamical aggregation of the least and the most mobile molecules. We find dynamical heterogeneity in supercooled water and string-like dynamics for the most mobile molecules. We also find the dynamical aggregation of the least mobile molecules. The two kinds of dynamical aggregation appear however to be very different. Characteristic times are different and evolve differently. String-like motions appear only for the most mobile molecules, a result predicted by the facilitation theory. The aggregation of the least mobile molecules is more organized than the bulk while the opposite is observed for the most mobile molecules.

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