Potential energy landscape contribution to the dynamic heat capacity

JOHN MCCOY, New Mexico Tech, JONATHAN BROWN, Ohio State University — The dynamic heat capacity of a simple polymeric, model glass former was computed using molecular dynamics simulations by sinusoidally driving the temperature and recording the resultant energy. The underlying potential energy landscape of the system was probed by taking a time series of particle positions and quenching them. The resulting dynamic heat capacity demonstrates that the long time relaxation is the direct result of dynamics resulting from the potential energy landscape.

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