Abstract Submitted
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Cole-Davidson Glassy Dynamics in Simple Chain Models[1] JOHN MCCOY, New Mexico Tech, JOANNE BUDZIEN, Sandia National Labs, TAYLOR DOTSON, New Mexico Tech, DOUGLAS ADOLF, Sandia National Labs, JONATHAN BROWN, New Mexico Tech — Rotational relaxation functions of the end-to-end vector of short, freely jointed and freely rotating chains were determined from molecular dynamics simulations. The associated response functions were obtained from the one-sided Fourier transform of the relaxation functions. The Cole-Davidson function was used to fit the response functions. For the systems studied, the Cole-Davidson function provided remarkably accurate fits (as compared to the transform of the Kohlrausch-Williams-Watts (KWW) function). The only appreciable deviations from the simulation results were in the high frequency limit and were due to ballistic, or free rotation, effects. The accuracy of the Cole-Davidson function appears to be the result of the transition in the time-domain from stretched exponential behavior at intermediate time to single exponential behavior at long time.

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