Orientational Relaxation in Simulated Polymer Melts TAYLOR
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FERNAN, New Mexico Tech — The orientational relaxation of simple poly-
mer chains was studied using second Legendre polynomial autocorrelation func-
tions. Such functions are commonly fit with a Kohlrausch-Williams-Watts (KWW)
stretched exponential form. The value of the stretching parameter, β, and the degree
that it changes as the glass transition is approached are both of physical interest.
In the current project, a novel approach to determining the value and variation of β
from molecular dynamics simulations is implemented. The methodology is found to
produce KWW fits of high accuracy. Moreover, the stretching parameter, β, is found
to collapse to a single-valued function of the decay timescale τ regardless of ther-
modynamic path. Connections are drawn to experimental results and theoretical
implications of the research are discussed.

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