Predicting the Viscosity of a Supercooled Liquid XI LIN, Boston
University — We present an atomistic description of the viscosity of a supercooled
liquid capturing the highly non-Arrhenius temperature variation for which no pre-
vious calculation has been given. A temperature dependent activation energy for
structural relaxation is derived by mapping the potential energy surface and extract-
ing saddle-point configurations and associated atomic coordinates. This essential
information is combined with the temperature variation of an effective local energy
minimum (inherent structure) to describe shear relaxation by thermal activation.
For a binary Lennard-Jones model the calculated viscosity shows a characteristic
crossover from strong (Arrhenius) to fragile (highly non-Arrhenius) behavior upon
appreciable undercooling, followed by a second crossover from fragile back to strong
behavior on approaching the glass transition temperature, both features we believe
to be generic. Analysis of atomic displacements associated with barrier crossing in
the fragile regime suggests a scenario of correlated motions along a chain of particles
as the underlying mechanism for slow viscous relaxation in glassy states.

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