**Designing Atomistic Simulation Workflows with MedeA®
A Case Study: Viscoelasticity of Glycerol at Ultra-high Frequencies**

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**Atomistic simulations are increasingly used to complement or enhance experiments**

Example: Nanoelectromechanical systems (NEMS) operating in liquid environments are of interest in biology.
- Resonance frequency increase into GHz and THz regime
- Same order of magnitude as atomistic/molecular relaxation processes in liquids such as water and glycerol
- Viscoelasticity becomes important
  - It is challenging to obtain relevant data via experiments
    - E.g., DMA (dynamic mechanical analysis) cannot probe GHz regime
  - Only one experimental study of $G'$ and $G''$ of glycerol at 25 GHz (shear) and 41.5 GHz (long.) – Nelson et al., JCP
    - Complex technique (TDBS)
    - Fluid structure not available
    - Difficult to gain insights into molecular motion
  - Molecular dynamics simulations offer alternative
    - We examined glycerol, a model simple viscous liquid, under ultra-high frequency shear and longitudinal deformation.
    - Many simulations needed to sweep temperature and frequency parameter space.

**Tools in MedeA® automate complex workflows and ease mundane tasks of initial configuration construction**

**Model construction and equilibration/production run protocols**

MedeA® Forcefields Module automatically assigns ff

MedeA Molecular Builder and MedeA® Amorphous Materials Builder are used for glycerol model constructions

Independent configurations created with MedeA® Amorphous Materials Builder are saved in structure list and ready for equilibration runs

**Tools in MedeA® automate complex workflows and ease mundane tasks of initial configuration construction**

**A Typical Workflow**

- Retrieving, viewing, and editing structures
- Selecting methods and programs
- Setting up computational parameters
- Performing calculations
- Analyzing results
- Storing results

**Results and comparison with experiments**

**Schematics of longitudinal and shear deformations**

Impose strain amplitude $\epsilon_0$ and $f$:

$$\epsilon(t) = \epsilon_0 \sin(2\pi ft + \delta)$$

Compute stress:

$$\sigma(t) = \sigma_0 \sin(2\pi ft + \delta)$$

$\sigma_0$ and $\delta$ are computed as a discrete Fourier transform (DFT) of stress magnitude and phase.

$$M'' = \frac{\sigma_0 \sin \delta}{\epsilon_0}$$

The shear modulus, $M''$, is calculated in a similar manner.

**Summary**

- High-throughput and high-fidelity modeling enabled by MedeA® provides guidance to screen large numbers of design options for materials before committing to experiments.
- MD is an effective tool for predicting the viscoelastic properties of simple liquids at ultra-high frequencies.

**References**


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