



MedeA Surface Tension

Ease the Tension in Surface/Interfacial Tension Calculations

At-a-Glance

The MedeA^{®1} Surface Tension module enables users to compute the surface and interfacial tension of a range of liquids, molten materials, and interfaces.

The underlying methodology computes the the difference between the average time of the stress components perpendicular and tangential to a liquid simulation slab.

Key Benefits

- Provides automated setup, execution, and analysis of LAMMPS molecular dynamics simulations for surface and interfacial tension calculations
- Handles model construction and assignment of forcefield atom types and charges in one unified environment so there is no need to use external tools
- Performs analysis of surface/interfacial tension with graphs showing convergence for a given simulation

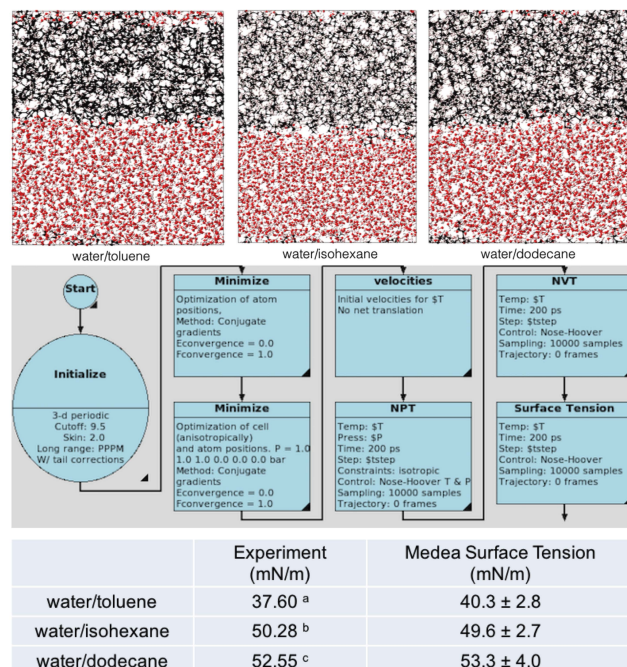


Figure 1: Interfacial tension of water/isoohexane, water/toluene, and water/dodecane interfaces from MedeA Surface Tension module using pccff+ forcefield compared to experimental values

Computational Characteristics

- MedeA Surface Tension module uses the LAMMPS classical molecular dynamics engine for efficient performance on computers from scalar workstations to massively parallel supercomputers.
- Accuracy depends on the quality of the employed forcefield. Use any of the supported forcefields in MedeA, import forcefields from literature, or even develop your own with MedeA Forcefield Optimizer.
- Works seamlessly with high-throughput techniques enabled by MedeA HT-Launchpad module to screen large number of design options of interfaces before committing to experiments.

'The MedeA Surface Tension module provides automated preparation, execution, and analysis of surface tension calculations - so you can focus on the science'

Required Modules

- MedeA Environment
- MedeA Forcefield
- MedeA LAMMPS
- MedeA JobServer and TaskServer
- MedeA Surface Tension

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Recommended Modules

- *MedeA Amorphous Materials Builder*
- *MedeA Diffusion*
- *MedeA Thermal Conductivity*
- *MedeA Viscosity*
- *MedeA EAM*
- *MedeA Forcefield Optimizer*
- *MedeA HT-Launchpad*

Find Out More

Learn more about the *MedeA Surface Tension* module from our [Materials Design Tutorials](#) page or by contacting info@materialsdesign.com:

- Interfacial Tension of Water and Organic Solvent Interfaces