MedeA Surface Tension

Ease the Tension in Surface/Interfacial Tension Calculations

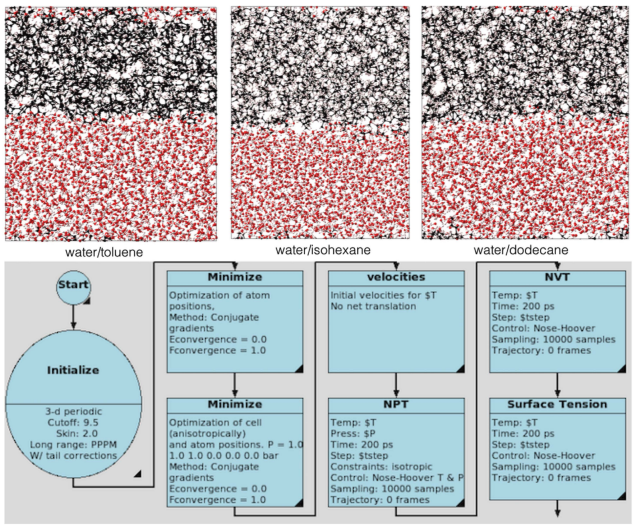
At-a-Glance

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



	Experiment (mN/m)	Medea Surface Tension (mN/m)
water/toluene	37.60 [a]	40.3 ± 2.8
water/isohexane	50.28 [b]	49.6 ± 2.7
water/dodecane	52.55 [c]	53.3 ± 4.0

Figure 1: Interfacial tension of water/isohexane, water/toluene, and water/dodecane interfaces from MedeA Surface Tension module using pcff+ 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*

[1] MedeA and Materials Design are registered trademarks of Materials Design, Inc.

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

12121 Scripps Summit Drive, Suite 160 San Diego CA 92131, USA
P: +1 760 495-4924 - F: +1 760 897-2179 - E: info@materialsdesign.com

materialsdesign.com

materials design