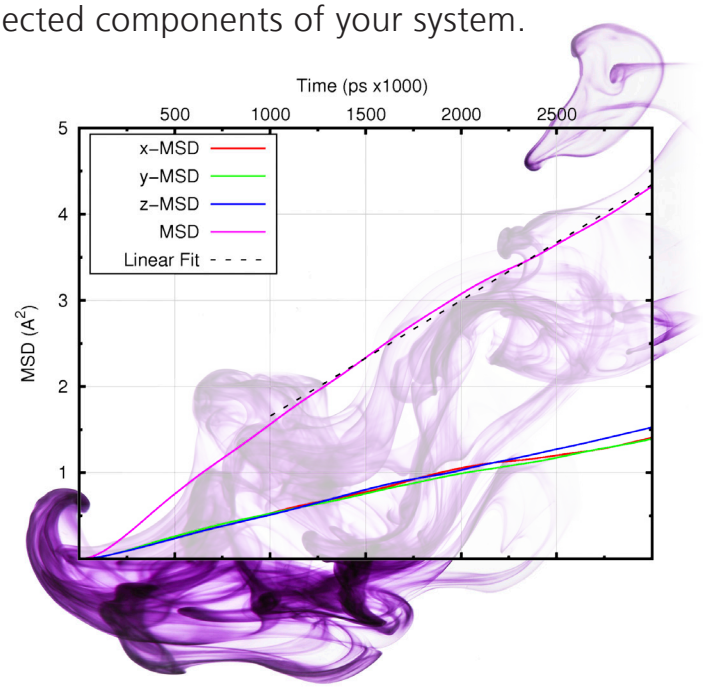
materials design

MedeA® LAMMPS-Diffusion

Diffusion controls a wide variety of processes and properties including manufacturing of semiconductor devices, environmental degradation of structural materials, corrosion, and oxygen permeability in polymers. The MedeA® LAMMPS-Diffusion module allows you to automatically compute the diffusivity of selected species using atomistic molecular dynamics techniques. At one glance, you see the diffusive behavior of selected components of your system.

Key Benefits of MedeA® LAMMPS-Diffusion:

- *Calculation of the mean squared displacement (MSD) of selected atom sets*
- *Determination of self-diffusion coefficients based on the Einstein diffusion equation*
- *Evaluation of calculation uncertainties*
- *Visualization and confirmation of the presence of the diffusive dynamics regime through the provision of log(MSD) versus log(t) plots*
- *Automated plot creation to facilitate analysis of calculation results*



Required MedeA® Modules

- *Core MedeA® Environment*
- *MedeA® JobServer and TaskServer*
- *MedeA® Forcefield*

Supported MedeA® Modules

- *MedeA® Polymer Builder*
- *MedeA® Mechanical Properties (MT)*
- *MedeA® LAMMPS-Thermal Conductivity*
- *MedeA® LAMMPS-EAM*
- *MedeA® LAMMPS-Viscosity*
- *MedeA® LAMMPS-CED*

Plug the MedeA® LAMMPS-Diffusion module into any LAMMPS simulation workflow and evaluate the diffusivity of selected system components. The MSD of selected atoms is computed with constant volume and energy (NVE). LAMMPS molecular dynamics and automated analysis of simulation results complete the workflow.

Load models from the MedeA® InfoMaticA database or popular file formats, create them with the MedeA® Amorphous Materials Builder, and even modify the models within simulation protocols of MedeA® Flowcharts.

Visit our website www.materialsdesign.com or contact your local Materials Design office for further information.

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