MedeA 3.2 features:

Improvements in structure **3D viewer**:

- Line antialiasing for high quality cell and line draw views
- Updated perspective projection for depth perception

- Numerous documentation enhancements, updates, and new tutorials
- *JobServer* job imports have been enhanced
- Enhanced graph plot file export functionality
- Added property variables for use in Flowcharts
- Enhanced labelling

Databases

- **New MSI Phase Diagrams Database** providing high-quality, evaluated phase diagrams, and related constitutional data

Builders and Editors

- **Thermosets:**
  - Support crosslinks between multiple types of site
  - Optional user-controlled connection probabilities
- **Mesoscale:**
  - Perform mapping of a coarse-grained onto an atomistic system
- **Nanoparticles:**
  - Improved algorithm, reducing particles build times for large systems

Engines

- ***MedeA VASP*:**
  - Automated calculation of energy of formation (VASP 6)
  - Excitonic effects in optical spectra from the model Bethe-Salpeter approach based on a model dielectric function
  - Use of ScaLAPACK through the Advanced/Restart tab
  - Listing of optical functions on a regular wavelengths grid in Job.out
  - Optical functions output as variables in workspace for use in Flowcharts
  - Addition of kinetic contribution to the average pressure obtained from molecular dynamics simulations
- ***MedeA LAMMPS:***
  - Distribution analysis available in LAMMPS Analysis
  - Group analysis available in LAMMPS Analysis
  - Pair Correlation analysis available in LAMMPS Analysis
- ***MedeA GIBBS:***
  - Enable the use of mesoscale forcefields (including MARTINI and SPICA)
  - Enable the use of EAM forcefields - allowing simulation of e.g. hydride formation
  - Use of 1-2/1-3/1-4 interactions as defined in the forcefield file (frc)
- ***MedeA* MOPAC**:
  - Updated version from Professor Jimmy Stewart

Property Modules

- ***MedeA QT:***
  - **New QT version:** v1.2.31 on linux and v1.2.30 on windows
  - Interactive correlation plot updates
  - Residuals plot for all correlations
  - All items on the Edit menu are disabled for the Models tab
  - Green check marks and gray hint boxes are restored on column menus for the Training Set tab
  - Plot menu items no longer appear on column menus for the Training Set tab
  - Plot menu items are enabled only for "Model N" columns on the Models tab
  - Additional logging capabilities have also been incorporated
- ***MedeA Phonon***:
  - Enable graphical display of thermodynamic functions, vibrational and electronic occupation contributions
  - Updated support for valence forcefields with LAMMPS
- ***MedeA MT:***
  - Enable graphical display of thermodynamic functions

Forcefields

- **PCFF+**: Forcefield extensions based on validated analysis for:
  - Extensions for ketones
  - Enhanced atom typing rules for selected systems
- Added **GAFF** (General AMBER forcefield, for organic molecules)
- Added **ReaxFF/CHONFClSi.frc**
- Updated **MEAM** descriptions

Analysis Tools:

- **New GUI** for assembling and plotting **thermodynamic functions** (from Phonon and MT)
- Additional handling of trajectory animations
- Automated video creation for animations

Fine control over frame selection for animations