MedeA 3.11 Release Note

Key features

- **Enhanced visualization with upgraded OpenGL support handling structures with hundreds of thousands of atoms**
- **Expanded Microstructure Builder with improved analysis tools and void creation capabilities**
- **Updated simulation engines including VASP 6.5.1 and LAMMPS 29Aug2024**
- **Advanced VASP Machine Learning ForceField (VASP MLFF) capabilities with refitting options and zone center phonon calculations**
- **New analysis tools including NMR chemical shift analysis, structural analysis flowchart stage and density profile analysis**
- **Implicit solvation options for all GAUSSIAN computations**
- **Improved PhaseField module supporting multiple diffusing species**

Builders and Editors and Visualization

- Extensive graphics improvements for accelerated and enhanced visualization of structures and surfaces. Optimized handling for structures containing hundreds of thousands of atoms.
- Several updates/enhancements for 3D rendering options
    - Depth cueing & fog thickness
    - Two modes of zoom: apply angular or positional zoom
    - Control of specular shininess

  - Polyhedra view
- Microstructure Builder
  - Implemented analysis of microstructure after building (grain volumes, occupations and misorientation angles)
  - Added option to facilitate the creation of voids
- Enhancements for 3D animator
- Supercell builder
  - Added option to the flowchart stage for creating an orthorhombic cell
  - Enhanced report printed in Job.out
- Docker: Enhancement for maximum displacement setting usage
- Several enhancements for robust building and compressing layers of polymeric and/or complex molecules (e.g. asphaltenes)
- New capability of building nanoparticles using input from Crystal Morphology (with/without open bonds)
- Enhancements for building Special Quasirandom Structures
- Enhancements for pair/triple and quadruple subsets

Engines

- **VASP**
  - New binaries (VASP 6.5.1)
  - Enhancements for MLFF related simulation protocols
  - Options for refitting MLFFs for improved performance
  - Enable calculation of zone center phonons applying MLFF
  - Enhancements controlling optical spectra obtained from advanced ab initio techniques

- **LAMMPS**
  - New binaries (Aug2024)

- **MOPAC**
  - Enabled use of variables in extra input
  - New ability to compute IR/Raman spectra and dynamics when frozen atoms are present

- **PhaseField**
  - Support for multiple diffusing species
  - Correlated (between species) bulk diffusion
  - Improved options for preconditioning
  - Improvements to GUI
  - Updated binaries

- **GAUSSIAN**
  - Implicit Solvation available for all computations, using a predefined or a new (custom) solvent
  - GUI enhancements

Forcefields

- **pcff+**
  - Enhanced forcefield assignment for n2o
  - Added templates for N2O and NO
  - Expanded support for phosphonium cations PR4+
  - Added coverage for orthoborate anion

Flowcharts

- New "Edit bonds" stage for bond editing inside a workflow
- New "Structural Analysis" stage

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Property Modules

- **UNCLE**
  - New UNCLE binaries with improved handling of symmetry when inactive sites are present
  - Structure lists with training data are now generated during cluster expansion optimizations
  - New Calculate Property stage to perform cluster expansion on a secondary property such as band gap, bulk modulus, and other scalar properties
  - Updates to the UNCLE save property stage to allow for more properties to be saved

- **Phonon**
  - Choose leading energy term for the thermodynamic functions from the Phonon GUI
  - Enhancements for Phonon simulations applying VASP's MLFF

- **Transition State Search**
  - Enhancement for running the Dimer Method applying VASP's MLFF

- **P3C**
  - The description of 'Dow Units' for permeability has been enhanced
  - The number of decimal places reported for polymer density, thermal conductivity (Tc), and refractive index (Ref) has been increased to three

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Analysis

- New NMR chemical shift analysis
- New Structural Analysis flowchart stage for HT usage
- New Density Profile analysis for single structures, structure lists and trajectories
- UNCLE Monte Carlo Temperature Profiles includes now color coding to distinguish between heating and cooling curves
- UNCLE Binary Ground State Diagram now allows for the switching of the y-axis property between total energy and pseudo heats of formation