MedeA 3.6 Release Note:

MedeA new features:

Description of MedeA 3.6 New Features and Enhancements

Engines:

- **VASP:**
  - Updated VASP executables to version 6.3.2
  - Full support for reuse of machine-learned forcefields (MLFF) obtained from previous molecular dynamics simulations for other VASP calculations and *MedeA* modules
  - Using the VASP GUI, reuse of MLFF descriptions are enabled for:
    - Single point calculations
    - Structure optimizations
    - Molecular dynamics simulations
    - Electron-phonon coupling
    - MT - Elastic properties
    - Property computations added for zone center phonons, work functions, and formation energies
  - Furthermore, reuse of MLFF descriptions are supported for modules such as
    - *MedeA Phonon*
    - *MedeA MT*
    - *MedeA TSS*
    - *MedeA UNCLE*
  - Enhanced reporting of calculation parameters for meta-GGA functionals
  - Updated entry field descriptions
  - Restore from previous job completed by PAW options control

- Updated user interface handling for L(S)DA+U parameters
- Additional SCF algorithm options supported for SCAN-rvv10

- **LAMMPS:**
  - Support for LAMMPS set cell stage remapping of atomic coordinates
  - Cohesive energy density stage enhanced for certain forcefields
  - Enhanced trajectory structure naming
- **GIBBS:**
  - Enhanced handling of phase composition in the *MedeA* interface
- **GAUSSIAN:**
  - IR and Raman spectra reports have been enhanced

Property Modules:

- **Phonon:**
  - Support reuse of machine-learned forcefields from VASP (MLFF) for evaluating all vibrational properties, such as phonon dispersion and energy density of states, thermodynamic functions, and non-electronic contributions to IR and Raman spectra
- **MT:**
  - Support for reuse of machine-learned forcefields from VASP (MLFF) to obtain elastic, mechanical and thermodynamic properties
- **TSS:**
  - Supports reuse of machine-learned forcefields from VASP (MLFF) to find transition states
- **Electronics:**
  - Re-enabled effective mass calculation from a previous VASP charge density task

- **UNCLE:**
  - Supports reuse of machine-learned forcefields from VASP (MLFF) for exploring configuration space
  - Improved handling of the user interface in absence of an active structure
- **InfoMaticA:**
  - Updated reporting of query result properties
- **Morphology:**
  - Enhanced linkage to surface builder

Flowcharts:

- Enhanced deformation optimization options for LAMMPS and VASP
- Optimized automated Job title handling
- Improved user interface support for keyboard short cuts
- Enhanced handling of flowchart description editing
- Compress layer stage enhancements
- General user interface enhancements
- New Surface Builder stage

Builders and Editors:

- **Updated Builders & Editors:**
  - Extensive general user interface enhancements and updates
  - Enhanced support for 4-coordinate pyramidal atoms
  - General usability enhancements
  - Substantial subset management enhancements

MedeA 3.6 Release Note:

- **Thermoset Builder:**
    - Enhancements for multisite systems and reaction probability support
- **Amorphous Materials Builder:**
    - Updated handling of input systems with active bonds
    - Improved handling of incorrectly bonded input systems
- **Surface Builder:**
    - Enhanced control of angular positioning
- **Mesoscale:**
    - Enhanced handling of the home path variable on Windows

Forcefields:

- **PCFF+:**
    - Accurate parameters for battery electrolyte systems including organic carbonates
- **MLPG:**
    - MLPG post-processing enhanced for NNP
    - MLPG enhanced SNAP hyperparameter optimization
    - Updated delta learning training set support
    - Enhanced SNAP .frc file description support
- **ForceField Optimizer (FFO):**
    - Enhanced reporting for spin polarized training set systems
    - Enhanced handling of validation set conditions
- **MEAM**:
    - Improved support for custom MEAM forcefields
- **General:**
    - Support for tabulated forcefields in LAMMPS

MedeA 3.6 Release Note:

Analysis Tools:

- Enhanced band structure plots for certain systems
- Export Band Structures and Densities of States on Windows:
    - Enable combined plots for large datasets and systems
- Export Phonon Dispersions and Densities of States on Windows:
    - Enable combined plots for large datasets and systems
- Enhanced animations of phonon modes from phonon dispersion plots
- Enhanced orbital view

Maintenance:

MD Maintenance: updated user interface for usability

JobServer & TaskServer:

Improved handling of inaccessible resources