MedeA 3.3 features:

Builders and Editors:

Edit cell

- Added option to switch between standard cell orientation and a preset arbitrary orientation

Supercell builder

- Option to rotate to standard orientation (default) or to preserve orientation according to cell construction

Thermosets

- Faster re-assignment of atom types (selective reassignment)
- Increased the number of sites supported in multi-sites crosslinking

Subsets

- Definition of subsets based on position criteria
- Extensions on the ability to transfer subset information upon system editing (copy/paste, merge, create supercells etc)
- Additional capability of freezing subsets via the Subset Manager stage
- Calculation of bond orders along with bonds
- Export to mol2 format for non-periodic and periodic systems
- Enhancements to exporting to pdb format

Engines:

VASP

- VASP 6.2.1 executables
- Automated procedure to calculate accurate optical spectra including excitonic effects via the Time Evolution approach
- Enhanced robustness of energy of formation and optical spectra simulations

LAMMPS

- Updated to the LAMMPS29Oct20 official stable version
- Supports NVIDIA GPUs on Windows
- Supports running on OpenMP threads on Linux and Windows
- Supports the PLUMED package on Linux

GIBBS

- GIBBS 9.7.4
- Improved handling of simulation output (configurations in pdb formats)
- Extended use of variables as simulation input (ideal gas heat capacity)
- Improvements on printed simulations' summary in Job.out

Forcefields:

MLP (Machine Learning Potentials)

- Access to a variety of published machine learning potentials for use with *MedeA LAMMPS*

MLPG (Machine Learing Potential Generator)

- Generation of machine learning potentials (on Linux and Windows)

Martini

- Addition of recently published Martini 3 for CG simulations

ForceField Optimizer (FFO)

- Enhanced support for fitting force and stress data
- Enhanced support for triclinic cells
- Improved performance for some forcefield classes

Property Modules:

Phonon and MT

- Enable automatic evaluation of the energy of formation for the system by *MedeA VASP 6*, thus providing temperature dependent energy of formation, entropy and free energy of formation

TSS

- Enable automatic evaluation of the energy of formation by *MedeA VASP 6* for initial and final configuration, as well as for all optimized transition states
- Various enhancements for performance

Electronics

- Enable automatic evaluation of the energy of formation for the investigated system by *MedeA VASP 6*

P3C

- Improvements in the calculation of 4 descriptors (Namide, Nco, Nhb, Nvkh) used in the calculation of Ecoh1 and Ecoh2