MedeA 3.0 features:

- A complete user interface (UI) refresh with updated icons, improved user experience with responsive dialogs, and enhanced operating system compliance on both Windows and Linux improving usability and enabling users to conduct cutting edge research with maximal efficiency,

- Builder capability extensions - facilitating the creation of complex crystalline and amorphous systems,
- A new module (Molecular Descriptors) - providing easy access to numerous topological and geometrical descriptors, in High-Throughput mode,
- Updates to the MedeA Forcefield library with new forcefield types and parameter sets and extensions broadening coverage and improving simulation accuracy,
- Use of reactive forcefields to simulate deposition and etching processes,
- Calculation and Analysis extensions for Optical Spectra - providing the ability to predict colors of metals

Description of *MedeA* 3.0 new features and enhancements

General

- New GUI theme, identical on Linux and Windows
- Enhanced high resolution and multi-screen support
- Full compatibility with previous *MedeA* releases
- Extensive and intensive documentation upgrades and updates
- Visualization: new options for lighting

Builders and Editors

- ***MedeA's* Molecular and Crystal Builders:**
  - Fragments attachment (e.g. for passivation of a surface)
- ***MedeA Amorphous Materials Builder:***
  - Coarse-grained systems support (use mass from forcefield file)
  - Updated orientation biasing for oriented film construction
  - Provision of both saved specific and immediate build options

Engines

- **MedeA VASP**
  - Updated work function results handling in Flowcharts
  - Enhanced support for optical spectra and color prediction
  - Drude conductivity for optical properties of metals
  - Automatic use of suitably fine energy grids for optical spectra calculations
- **MedeA LAMMPS**
  - Improvements for switching between 3D and 2D periodicity
  - Default variables in all LAMMPS stages
  - Added support on NVIDIA GPUs
- **MedeA GIBBS**
  - Complete final system update via .sci file
- **MedeA MOPAC**
  - Custom stage for fully customized MOPAC simulations
  - Extra Input enabled for all MOPAC flowchart stages

Property Modules

- **MedeA Electronics**
  - Access to the energy increment for numerical integration from the GUI of MedeA Electronics to fine-tune transport properties
  - Automated positioning of the Fermi level into the center of the gap for the derivation of transport properties
  - Additional transport functions: electronic fitness functions, inverse transport effective masses
- **MedeA QT**
  - Complete handling of datasets with non-existing descriptors
  - Updated multi-row selection and editing capabilities
- **MedeA Deposition**
  - Ability to use reactive forcefields to simulate deposition and etching processes

- **MedeA ForceField Optimizer (FFO)**
  - Added support for ReaxFF potential
  - Improvements for Tersoff potential optimization

High-throughput

MedeA HT-Descriptors (New)

- *HT-Descriptors* for molecular species can now be easily calculated for the members of a structure list and used in creating QSPR/QSAR correlations, using MedeA QT.

Forcefields

- **pcff+ : Forcefield extensions for:**
  - Al2O3
  - alkyl-arsines
  - Carboxylic esters
  - cloro/fluoro hydrocarbons (HCFCs)
  - graphene oxide
  - silica-siloxane interfacial regions

- **TraPPE-UA+: Forcefield extensions for:**
  - cyclic hydrocarbons
  - alkyl-arsines
  -
- ***MedeA COMB3 & MedeA ReaxFF*: addition of descriptions and parameters

Analysis Tools

- ***MedeA's* Optical Spectra**
  - Automatic differentiation between optical properties of metals and semiconductors/insulators, as identified by VASP post-processing
  - Automatically retain the Drude conductivity from VASP post-processing

- Automatically add Drude term for metallic systems, making use of the default Drude conductivity as calculated by VASP
- Added transmission coefficient as a function of wave length and slab thickness
- Attenuation and absorption coefficient
- Enable customization of energy/wavelengths units
- Visual color prediction upon reflection and transmission, for direction dependent optically anisotropic materials
- CIE 1931 and 1964 color spaces upon reflection and transmission (direction dependent in case of optical anisotropy)

MedeA's JobServer & TaskServer

- Enhanced *MedeA* JobServer performance (asynchronous, non blocking mode)
- Extensions for HTTPS support