Release notes

Contents

1 *MedeA* 3.0

The *MedeA* 3.0 release features a complete user interface 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.

This *MedeA* release continues the Materials Design tradition of providing the highest quality materials science simulation capabilities based on investment in science, software, and infrastructure; and depending on the Materials Design culture of innovation and dedication to technical understanding.

The key areas of development in the release are as follows:

1.1 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

1.2 Builders and Editors

- Fragments attachment (e.g. for passivation of a surface)
- Amorphous Materials Builder:
- Coarse-grain systems support (use mass from forcefield file)
- Updated orientation biasing for oriented film construction

- Provision of both saved specific and immediate build options

1.3 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 (Drude term)
  - 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

1.4 Property Modules

- Electronics:
- Access to the energy increment for numerical integration from the GUI of Electronics to fine-tune transport properties
- Automatically shift 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
- QT:
  - Complete handling of datasets with non-existing descriptors
  - Updated multi-row selection and editing capabilities
- Deposition:
  - Using reactive forcefields to simulate the materials science processes of both deposition and etching processes
- ForceField Optimizer:
  - Added support for ReaxFF potential
  - Improvements for Tersoff potential optimization

1.5 High-Throughput

- Molecular Descriptors (New): Descriptors for molecular species can now be easily calculated for the members of a structure list and used afterwards for creating QSPR/QSAR correlations, using MedeA QT. These descriptors include:
  - topological

  - geometrical

1.6 Forcefields

- pcff+: Forcefield extensions based on validated analysis 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
- COMB3 & ReaXFF: addition of descriptions and parameters

1.7 Analysis Tools:

- Optical Spectra:
  - Automatic differentiation between optical properties of metals and semiconductors/insulators, as identified by the 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 functions of wave length and slab thickness
  - Attenuation and absorption coefficient
  - Enable customization of energy/wavelengths units
  - Visual color prediction upon reflection and transmission, for optically anisotropic materials direction dependent
  - CIE 1931 and 1964 color spaces upon reflection and transmission (direction dependent in case of optical anisotropy)

1.8 JobServer & TaskServer

- Enhancements JobServer performance (asynchronous, non blocking mode)
- Extensions for HTTPS support