Release notes

Contents

1 *MedeA 3.6* 6 December 2021

1.1 Builders and Editors:

- Updated Builders & Editors
- Addition of controls on each system-view window
- Easy access to 3D viewing options through the controls on the system-view window
- Addition of visual aids / enhancements, such as: - Depth cueing - Control of perspective view - Lighting options - Creation of user-defined profile controlling 3D viewing options - Axes and axes labels and positioning control
- Introduction of right-panel with “switch” mode for access to multiple panels
- Replacement of a number of “floating windows” with right panel (e.g. edit cell/symmetry, supercell builder etc)
- Update of “Docking” tool, including view of energies and ability of selection of any created configuration
- Geometric Analysis as a side-panel on the structure-view window (periodic systems)
- Several enhancements in the Trajectory animations, including: - Increase of rendering speed - Improved efficiency in bond handling - Improved control of viewing (mixed view) - Animation panel on the trajectory animation window - Smart access restriction to trajectories
- Structure Lists’ animation, including plotting of properties and descriptors that are included / saved therein

1.2 Engines:

- VASP: - Speed-up of parsing large OUTCAR files as created by long molecular dynamics simulations
- GIBBS: - Calculation of sorption grids within the GCMC computation
  - speed up (parallelized building of grids)
  - decrease of JS/TS traffic (no need for grids’ transfer)
  - automated rebuild of grids if deleted or inappropriate
  - increased consistency (grids’ build and simulation run using a single set of binaries)

DOCUMENTATION

1.3 Forcefields:

- MLPG: - Addition of neural network potentials by adding n2p2 to the MLPG - Efficient inclusion of post-DFT approaches by using “Delta learning” - Bond length, bond angle and torsion angle distribution analysis in the MLP data manager
- PCFF+: - Refined parameters for trialkyl phosphates

1.4 Property modules:

- Phonon: - Enhanced analysis of Infrared and Raman spectra
  - specify experimental conditions (polarized or unpolarized light / monocrystal or polycrystalline sample)
  - for Raman spectra: specify incident and scattered light orientation and polarization orientation
  - display Raman cross section or Raman reduced spectra, handle the temperature (Bose) factor
  - Enhanced analysis of thermodynamic functions - analyze contributions of atoms in Cartesian directions to the thermodynamic functions - analyze thermal displacements of atoms as a function of temperature