Release notes

Release Notes

Contents

MedeA 3.7.0 April 2023

The MedeA 3.7.0 release provides new capabilities for vibrational analysis based on molecular dynamics trajectories, updated VASP executables (6.4.1) with full integrated MedeA support, extensive enhancements in Machine Learning based simulation, and a broad array of general improvements to the entire MedeA environment.

An overview of updates in this MedeA release is provided below.

1 Builders and Editors:

- **Subsets:**
  - Additional capability to select complete molecules through the “extend selection” option
  - Targeted performance enhancements for large number of atoms
  - Enhancements for editing subset coloring
  - Enhancements for subset splitting capabilities
  - Enhancement in the Subset Overview panel
  - Addition of an elements option to the attach fragments functionality
- **Thermosets:**
  - Enhancements for controlling the conversion extent
- Enhancements for import of structures in extended xyz format
- Enhancements for import of large PDB structures
- Gnuplot update (5.4.6)
- New functionality for the deletion of overlapping atoms in a defined selection
- Enhancements in handling of mesoscale structures in the supercell builder
- Enhancements for Interface builder
- Three additional popular atom color schemes added

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2 Engines:

- **VASP:**
  - VASP 6.4.1 executables with integrated MedeA support (NEW)
  - Site-specific output of NMR chemical shift data
  - Addition of chemical shift data and magnetic susceptibility to the workspace
  - Enhancements for output of EFG, Hyperfine parameters, and Born effective charges
  - Upgraded POSCAR files containing elements and atom-site correspondence
  - Return status given in structure lists and trajectories, enabling easy convergence assessment for large datasets
  - **MLFF enhancements:**
    - Enabling MLFF-based forces in trajectories
    - **Creation of a separate MLFF_TrainingSet.sli structure list with significant, ab initio-calculated s** (e.g. for further use in machine-learning applications and forcefield fitting)
    - Addition of Bayesian Error and RMSE Analysis in graphical form for VASP-MLFF
    - Reduced MLFF OUTCAR data volume via trajectory file frequency for swift post-processing and trajectory creation
- **LAMMPS:**
  - LAMMPS 2Jun2022 executables (NEW)
  - Automatic selection of correct executable for extended GPU support
  - Addition of Nose-Hoover-Andersen in list of control temperatures in LAMMPS NVT/NPT stages
  - Enhancements form minimization stage under pressure
  - Enhancements for restoration of United-Atom hydrogens for carbon atoms of unsaturated hydrocarbons
- **GIBBS:**
  - Several updates/enhancements to GIBBS trajectories and generated structure lists
  - Enhancement in improper torsions' input
  - Extensions for handling and reporting of 1-2/1-3/1-4 interactions in GIBBS
- **MOPAC:**
  - Enhancement for calculating thermodynamic properties for a single temperature in a Thermodynamics stage

3 Forcefields:

- **MLPs & MLPG:**
  - Support for ACE MLPs (in LAMMPS, CPU & GPU) (NEW)
  - Full user control of hyper-parameter convergence tolerance
  - Checking and recording of status for VASP calculations

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  - Enhancements on data handling
- Extensions for tabulated forcefields
- **PCFF+:**
  - Introduction of unique atom types for inorganic sulfate anions

4 Property modules:

- **P3C:**
  - Refined 5 membered rigid rings recognition and contribution in P3C in consultation with Dr. Jozef Bicerano
  - Updated P3C tab in Molecular Builder for repeat units containing over 100 atoms, allowing application of P3C computation on demand
  - Enhanced handling of repeat units with common head and tail atoms
  - Enhanced handling of silane based repeat units
- **Electronics:**
  - Calculation and graphical presentation of carrier mobility (NEW)
- **PhononMD: (NEW)**
  - Vibrational density of states and its partial contributions from molecular dynamics velocity autocorrelation functions
  - Automated plot creation facilitating analysis of results
  - Vibrational thermodynamic properties such as internal energy, entropy, Helmholtz free energy, and heat capacity

5 Citations/References:

- New link in “Help” menu in MedeA that points to the “How to cite” section in the MedeA manual
- Downloadable ris/bibtex references for MedeA and MedeA tools/modules

6 JobServer & TaskServer:

- Enhancements for downloading structures from the JS containing spaces in their names
- Addition of warnings if GPU requested but not present on the TaskServer
- New capability for automated zip file creation and download