MedeA 3.7 Release Note:

MedeA new features:

Description of MedeA 3.7 New Features and Enhancements

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

MedeA 3.7 Release Note:

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 structures/data (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

Forcefields:

- Enhanced deformation optimization options for LAMMPS and VASP
- Optimized automated Job title handling
- Improved user interface support for keyboard short cuts
- Enhanced handling of flowchart description editing
- Compress layer stage enhancements
- General user interface enhancements
- New Surface Builder stage

Builders and Editors:

- **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
- Enhancements on data handling
- Extensions for tabulated forcefields

- **PCFF+:**
  - Introduction of unique atom types for inorganic sulfate anions

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

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

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
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