Release notes

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

1. Builders and Editors:
   - Microstructure Builder (New)

     The MedeA Microstructure Builder creates microstructure models for atomistic simulations using a Seed & Growth algorithm with starting points either placed randomly or at user-specified coordinates within a supercell. Each such point is used as an origin to grow a crystalline grain by adding atoms from that seed point outwards until a grain boundary is encountered.

     The models created by the MedeA Microstructure Builder can be used with other MedeA tools to explore the structural, energetic, and dynamic characteristics of microcrystalline materials.
   - Enhancements for exporting structures to extxyz
   - Enhancements for bond computation
   - Enhancements for assigning element colors
   - Addition of the ability to use a variable for density in the amorphous builder stage
   - Added an automated orthorhombic construction mode to the Supercell Builder. This functionality is made available if the active structure is non-orthorhombic.
2. Engines:
   - VASP:
     - VASP 6.4.2 executables for Linux and Windows
     - Structure optimization: all combinations of constraints for atom positions, cell volume and shape are available
     - Added support for several Molecular Dynamics features through the user interface:
       * The microcanonical ensemble can be executed in two ways, one is consistent with older VASP versions
       * Canonical ensemble (nVT) ensemble: users can now choose Nose-Hoover, Andersen, and Langevin thermostats and their parameters
       * Added isoenthalpic isobaric (nPH) ensemble (New)
       * Added lattice constraints and monitoring for the isothermal isobaric (nPT) and isoenthalpic isobaric (nPH) ensembles. The options are:
         · isotropic
         · fixed lattice angles

DOCUMENTATION

        - constrained
        - unconstrained
    - Short access time when loading machine-learned forcefields
    - New calculation type to refit machine-learned forcefields:
        - for fast running applications, or
        - with Bayesian error prediction, or
        - with reselected local reference configurations
    - New user interface for fine-tuning the on-the-fly machine learning process and the refitting of forcefields. For instance:
        - thresholds for Bayesian errors of forces and their updating process
        - thresholds for configurations and sparsification
        - relative fitting weights of energy, forces and stress
        - atomic reference energies
        - definition of descriptors and the basis set expansion
        - output options
    - Versatile trajectory creation, in particular for MLFF based molecular dynamics and on-the-fly learning
    - Updated gnuplot graphics for machine learning
    - Improvments for return status handling
    - Enhancements for band structures based on non-local functionals without range separation
    - Adapt low scaling GW to VASP 6.4.2 executables
- LAMMPS:
    - Update of automatically produced plots (post-processing)
    - Addition of option for writing a trajectory in native LAMMPS format
    - Addition of warning if there are frozen atoms during an NPT run
- GIBBS:
    - GIBBS 9.7.8 executables for Linux and Windows
- GAUSSIAN:
- Optimization of transition states accessible in flowcharts

3. Forcefields:
    - MLPG:
        - Enhancement to allow for manual assignment of structures to training/validation sets
        - Addition of “Coordinates” property when importing into the Fitting Data Manager
    - Enhancements on forcefields handing in FFO
    - PCFF+:
        - Refined nonbond parameters for carbon in acetal groups
4. Property modules:
    - Polymer Expert (New)

      The Polymer Expert is a new module in the MedeA environment in MedeA 3.8. The innovative Polymer Expert capability facilitates de novo polymer design through high-efficiency access to a

substantial (>1.1 million entries) database of polymer properties, PEARL (Polymer Expert Analog Repeat unit Library). Polymer Expert allows you to identify novel polymers by querying the PEARL database based on properties and property ranges. You can also search for biologically derivable analogs within the PEARL database. Polymer Expert was developed in collaboration with Jozef Bicerano the author of Prediction of Polymer Properties, Marcel Dekker, Inc. (2002) and is described in the paper (J. Bicerano, D. Rigby, C. Freeman, B. Leblanc, and J. Aubry, Polymer Expert - A Software Tool for De Novo Polymer Design, 2023 - which has been submitted for publication).

- P3C:
  - In consultation with Jozef Bicerano, a variety of upgrades to P3C have been made in the MedeA 3.7.1, 3.7.2, and MedeA 3.8 releases. In particular:
    - The naming of mechanical properties has been updated to clarify the temperature of the properties reported by P3C.
    - Mechanical properties are generally reported at 298K. When a polymer has a computed glass transition temperature (Tg) below 298K, the Young's modulus (Eyoung298K), shear modulus (Gshear298K), and the shear yield stress (Sy298K) are set to -1.0 so as to avoid providing misleading properties.
    - The bulk modulus (B298K) is computed using correlations which account for low Tg (lower than 298K) materials and incorporates a transition region for materials with Tg's close to 298K.
    - The Poisson ratio, vpoisson298K, is computed for materials with Tg's greater than 298K using a simple correlation, and for materials with Tg's lower than 298K for the onset of the rubbery region for that polymer.
    - Two new properties, EyoungTgp30K and GshearTgp30K, are now reported. These are the Young's modulus and shear modulus at the onset of the rubbery region, i.e. 30K above the polymer's Tg.
    - Property descriptions have been updated to reflect the enhancements to mechanical property reporting described above.
    - Properties are now reported with 2 decimal places, except for the Poisson ratio, which is reported with 4 decimal places.
    - An additional Critical molecular weight property - using an alternative correlation described in Jozef Bicerano's Prediction of Polymer Properties, Marcel Dekker, Inc. (2002) has been implemented.
    - The thermal expansion, aT, has been updated to make this property a continuous, rather than discontinuous, function of Tg.
    - A number of descriptor enhancements have been incorporated improving property prediction accuracy.
    - Systems with more than 100 atoms may now be treated by P3C in the interactive P3C panel, upon user request.
    - P3C no longer provides results for systems containing phosphorous and iodine, as repeat units containing these elements were not available during the original parameterization of P3C.
    - Predictions for polymers with just silicon and nitrogen on the backbone, e.g. poly(dimethyl silazane), have been enhanced.
    - Thermal conductivity, Tc, has been added to the properties computed by P3C
    - The handling of the output of gas permeabilities has been enhanced.
    - The treatment of rotatable bonds in siloxane alkyl side chains has been enhanced, based on input from Jozef Bicerano, to improve the predictive capabilities for such systems.
    - In general, predicted Tg values below 100K represent extrapolation significantly below the bottom of the range of data used in developing the P3C equation. Accordingly, when

P3C might compute a Tg<100K for a given repeat unit it now provides a report stating that this repeat unit is outside of the current applicability range of P3C.

* Similarly, elastic moduli are never negative in practice. If P3C calculates one or more negative moduli, because the input descriptors are outside of the ranges employed in the development of P3C's correlations, it provides a message stating that the repeat unit is outside the current applicability range of P3C.
* Enhancement for interactive computation for large repeat units (on-demand)

- Deposition:
  - Enhancements for subsets used in deposition
- MT:
  - Short access time when loading machine-learned forcefield
  - Output enhancements

5. Analysis:
   - Enhancement for pair correlation panel
6. Infrastructure:
   - Addition of the MedeA Python environment
   - Update of IntelMPI to 2019 version on Linux