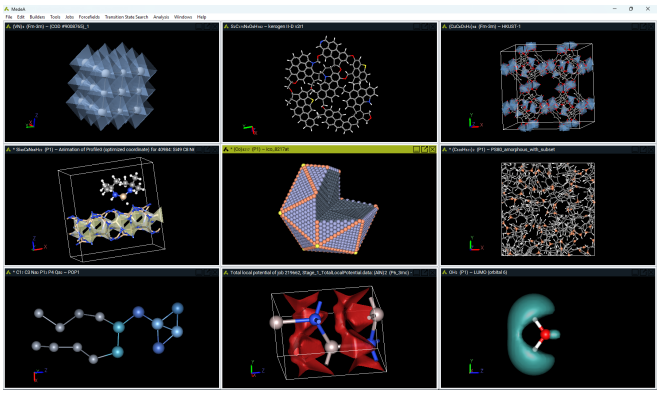
What's New in MedeA 3.13

Atomic Insights at Scale

Materials Design announces *MedeA*®[1] 3.13, the latest release of its comprehensive materials simulation environment, delivering significant advances across model building, simulation, and analysis. This release brings atomic insights at scale — empowering researchers to tackle larger, more complex systems with greater speed and confidence.



MedeA *3.13 - Atomic Insights at Scale*

A major addition is the new *MedeA ML Property* module, enabling rapid property prediction through machine-learned potentials for large-scale systems beyond the reach of conventional DFT calculations. There are major enhancements to structural builders with improved validation and visualization, advanced analysis tools for comprehensive materials characterization, and a new export feature for improved compatibility with the OVITO visualization platform.

The highly anticipated update to VASP 6.6.0 offers a new and very accurate NMR chemical shift computation for solids within the so-called ZORA approximation. The *MedeA* VASP interface now features access to new solvation models for studying solvated systems and much enhanced visualization of the electronic structure of solids, with new bandstructure projections and interactive Brillouin zone rendering. The enhancements to bandstructure visualization benefit *MedeA* Phonon users as well. Also highly relevant to VASP users: full UI support and access to additional transition state search methods via the TSS module.

At the continuum end of the multiscale offering, this release continues the rapid evolution of the powerful *MedeA PhaseField* module, which now allows the modeling of nucleation, fracture, boundary elementary reactions, phenomena relevant to Li-ion batteries, and much more.

At-a-Glance

Key Features of MedeA 3.13

- **ML Property Module (NEW)**: Groundbreaking new module to direct prediction of atomic-scale properties for large-scale systems beyond the reach of conventional DFT calculations using a machine learned approach
- **VASP 6.6.0 Integration**: New binaries with more accurate NMR chemical shift computations, enhanced optical spectra and projection data handling, and improved band structure visualization with interactive Brillouin zone rendering
- **Phasefield Module**: Enhanced capabilities for modeling nucleation, fracture, boundary elementary reactions, and other phenomena
- **Transition State Search (TSS)**: Full access to established VASP and VTST methods with comprehensive documentation and support
- **Enhanced Builders**: Improved amorphous structure generation, random perturbation display, input validation for slabs, and surface generation enhancements

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- **Advanced Analysis Tools**: Enhanced band structure and phonon dispersion rendering, improved geometric pair subset analysis, extended projection data handling with element filtering and aggregation capabilities
- **OVITO Export**: New export feature for improved compatibility with OVITO visualization platform
- **Extended Engine Support**: LAMMPS ReaxFF preprocessing enhancements and GIBBS 9.8.3 binary with updated scripts

Clive Freeman, CEO of Materials Design comments:

This release marks a major step forward in accelerating process optimization and discovery through advanced simulation and machine learning. At the heart of this release is the new AI-based ML Property module, which allows researchers to quickly predict properties such as charges, core-level energies, electric field gradients, and partial electronic densities of state, even for systems beyond the scope of traditional first-principles methods. Alongside the innovative ML Property module, this release introduces enhanced structural builders, expanded transition state search capabilities, and powerful new analysis tools. Together, these features enable users to explore increasingly complex materials problems with greater confidence, speed, and precision. As Richard Hamming noted, the purpose of computing is insight. This principle guides our development. The MedeA productivity environment helps you efficiently extract the insights needed to advance your research.

About Materials Design:

Materials Design, Inc. is the leading atomistic modeling and simulation software and services company for materials. Materials Design helps customers across diverse industries design and optimize materials and processes, predict materials properties, and generate value through innovation. The company is dedicated to providing efficient access to the world's leading atomistic and electronic scientific simulation methods.

The advanced MedeA®Page 1, 1 materials modeling and simulation environment is used by thousands of customers at more than 800 institutions worldwide. Scientists and engineers in industry and research institutions rely on the MedeA Environment to simulate materials properties and understand diverse phenomena. The MedeA Environment enables users to create better products while saving valuable research and development time and cost.

The MedeA Environment integrates world-leading structural databases (totaling over 1.2 million entries), electronic structure engines (VASP, Gaussian, MOPAC), molecular dynamics (LAMMPS), Monte Carlo methods (GIBBS), and Continuum methods (PhaseField) with a host of powerful building, editing, and analysis tools in a unified environment, allowing the creation of efficient workflows. Its innovative high-throughput (HT) capabilities enable the use of computational resources to achieve exceptional results.

Overview of *MedeA* 3.13

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

Builders and Editors

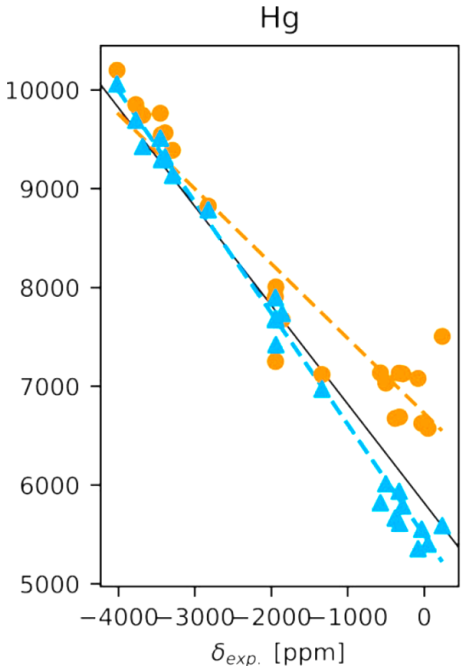
- Amorphous Materials Builder
  - Enhancement of amorphous structure generation capabilities
- Random Perturbation Builder
  - Enhancement of bond display for significantly perturbed structures
- Microstructure Builder
  - Enhancement of input validation for slabs with distance verification
- Surface Builder
  - Enhancement of surface generation and rendering
- Subset Manager GUI

- Enhancement of graphical interface for subset management

Engines

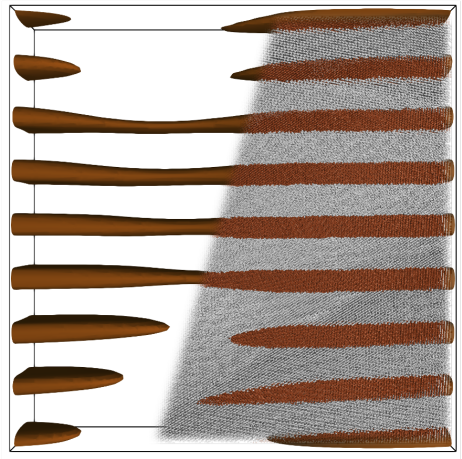
- VASP
  - New VASP 6.6.0 binaries
  - New VASPsol++ linear and local implicit solvation model as an alternative to the original VASPsol model
  - New VASPsol++ nonlinear and nonlocal implicit electrolyte model as a further option
  - New CP-VASP for DFT calculations at constant electrode potential, grand canonical ensemble for electron dynamics
  - Added spin-orbit coupled or scalar-relativistic zeroth-order regular approximation (ZORA) for NMR chemical shielding computations
  - Added nucleus-independent chemical shielding (NICS) tensor calculation at off-nucleus positions
  - Added output of NMR current response to an external magnetic field
  - Added support for NMR data in MAGRES format for post-processing
- LAMMPS
  - Enhancement of ReaxFF preprocessing for wildcard handling
    - Improved handling of angles, torsions, and hydrogen bonds
  - Improvement in custom forcefield loading
- GIBBS
  - New GIBBS 9.8.3 binaries
- PhaseField
  - Fracture support
  - GUI support for nucleation
  - Classical nucleation theory (nucleation rates)
  - Integrators for bulk and grain boundary elementary reactions (trapping and catalysis)
  - Dendrite support for two-phase problems for solidification and lithium-battery applications
  - VTS compositional eigenstrain via CLI
  - Partial assembly to reduce memory for 3D problems
  - Major speedup for elastic problems (Voigt tensor change)

[2] T. Speelman et al., J.Chem. Phys. **145**, 104115 (2025)



Calculated vs experimental NMR chemical shifts for mercury compounds, using the VASP ZORA approximation. The circles correspond to scalar relativistic and the triangles to spin-orbit coupling (SOC) levels of theory. The SOC predictions are very close to the experimental data (solid line depicts the ideal slope)[2].

  - Electrochemistry support via CLI
  - Piezoelectric coupling via CLI

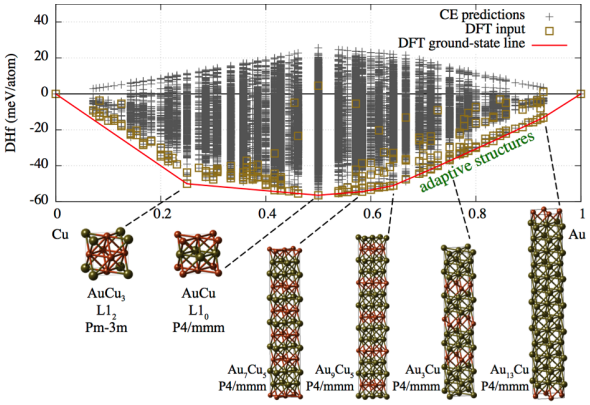


Lamellar structure in spinodal decomposition.

Property Modules

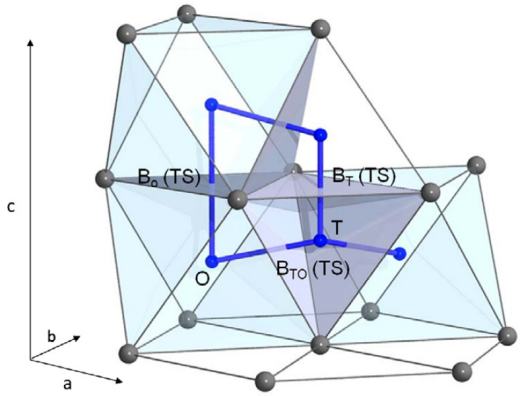
- ML Property (NEW)
  - Direct property prediction for large-scale systems beyond the reach of conventional DFT using a machine learned approach
  - Rapid calculation of atomic-scale properties:

    - Partial electronic charges
    - Core level energies
    - Electric field gradients
    - Partial electronic density of states (DOS)
  - Efficient batch processing of structure ensembles
  - Systematic property screening capabilities
- Phonon
  - Improvement in symmetry-related guidance and messaging
- UNCLE
  - Added random number generator seed input for improved reproducibility of results



Ground-State Phase Diagram of the Au-Cu System from Cluster Expansion

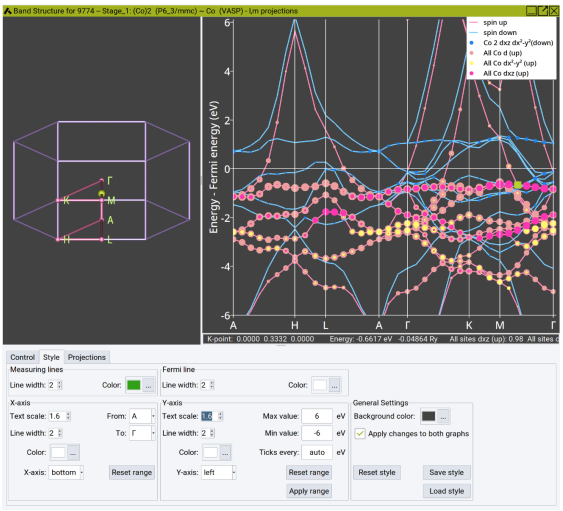
- Transition State Search (TSS)
  - Full access to well-established native VASP and VTST transition state search implementations already used by many VASP standalone and expert MedeA users
  - Complete integration of these methods in MedeA's processing, post-processing and energy profile analysis
  - Increased convenience for running on high-performance computing centers
  - All transition state search techniques are fully documented and supported on Linux and Windows
  - Additional Solid-State Nudged Elastic Band method offered by VTST



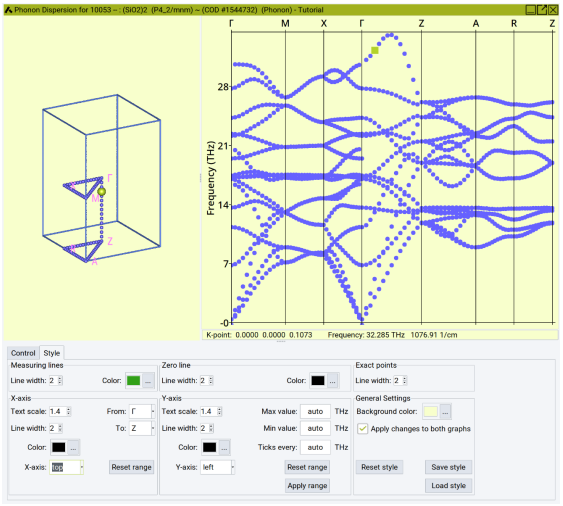
Interstitial diffusion pathways in hcp-Zr

Analysis and Post-Processing

- Structural Analysis
  - Enhancement of geometric analysis of pair subset distributions
- Electronic Band Structure
  - Enhancements to band structure plots
    - Added an interactive 1st. Brillouin zone visualization indicating the k-point path for improved clarity and understanding of the band structure
    - Improvements to style and formatting of band structure plots for increased customizability of the presentation
  - Improvements in band structure handling of projection data
    - Support for l,m-projections on atoms
    - Automated summation of multiple sites of the same element
    - Customizable summation of projection data for aggregation
    - Filtering of projection data by site/atom, element, and custom summation
    - Addition of capability to normalize projection data to atomic contributions
- Phonon Dispersion
  - Enhancement of phonon dispersion rendering
    - Added an interactive 1st. Brillouin zone visualization indicating the k-point path for improved clarity and understanding of the phonon dispersion
    - Improvements to style and formatting of phonon dispersion plots for increased customizability of the presentation



Band structure plot containing l,m-projections with interactive 1st. Brillouin zone visualization



Phonon dispersion plot with interactive 1st. Brillouin zone visualization

- PhaseField Visualization
  - Addition of dedicated 2D OpenGL viewer infrastructure for improvement in PhaseField visualization

Forcefields

- ReaxFF wildcard handling for angles, torsion, and hydrogen bond terms has been enhanced.

General Improvements

- New OVITO export feature for improvement in compatibility with OVITO visualization. Exporting to OVITO is now available for all *MedeA* single structures, as well as trajectories and structure lists.
- Extension of plot generation capabilities for ACE machine learning potentials
- Added support for SVG export to the various plotting tools
- Improved export of *MedeA* plots to CSV and text files