MedeA Materials Modeling Environment

At-a-Glance

With *MedeA*®[1] use simulation and correlation methods to:

- Predict the physical and chemical properties of materials, and
- Study the mechanism(s) that govern micro and macroscopic phenomena

The *MedeA Environment* is designed for:

- High Performance, with high productivity integrated tools
- Property Prediction using application-specific property modules in conjunction with state-of-the-art simulation engines
- Use of Reproducible Workflows as graphical flowcharts for multi-stage protocols that can be stored and re-applied
- Efficient use of computational resources
- High Throughput flowcharts for automated mapping and screening
- Customization for diverse applications

Key Benefits

- Accelerate materials design, scientific discovery, and productivity through the use of High Throughput tools within reproducible Workflows
- Unlimited job submission and management with no core counting, at no additional cost

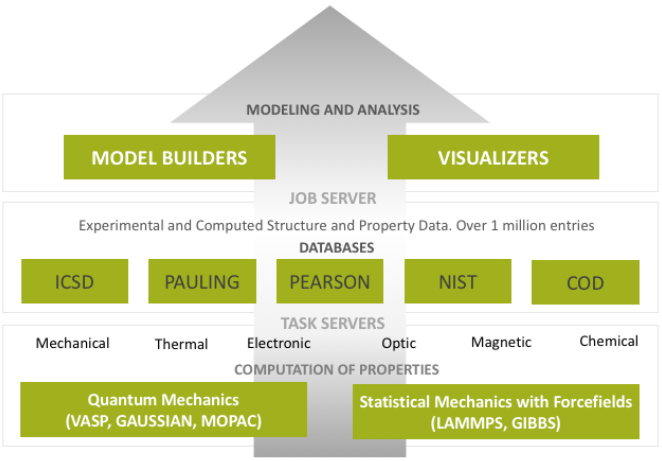
Designed to Perform

MedeA is designed for materials engineers and scientists requiring rapid and reliable solutions for a range of materials issues related to application areas, such as power generation, automotive applications, energy storage, alloy design and optimization, micro-electronics, chemicals, and petrochemicals.

[1] MedeA and Materials Design are registered trademarks of Materials Design, Inc.

Academic researchers rely on *MedeA* as a basis for research in computational materials science, and for interpretation of experimental data, providing understanding of materials' properties. *MedeA* is an invaluable tool for education and educators.

Created for high productivity, *MedeA* helps you focus your materials research and development, using graphical workflows, automated analysis, and high throughput computation tools. Team interaction and collaboration are facilitated through the use of Flowcharts, as well as open access to simulation input and output through the *JobServer MedeA* architecture.



'Created for high productivity, MedeA helps you to boost your materials research and development'

Architecture

MedeA embeds modules in a core framework with components that can be installed on a single machine or distributed over a network of computers, including large scale supercomputers.

MedeA has a unique 3-tier architecture that offers flexibility, and optimizes the use of available computing resources, while reducing the human time and effort involved in simulation deployment. This 3-tier architecture comprises the following key elements:

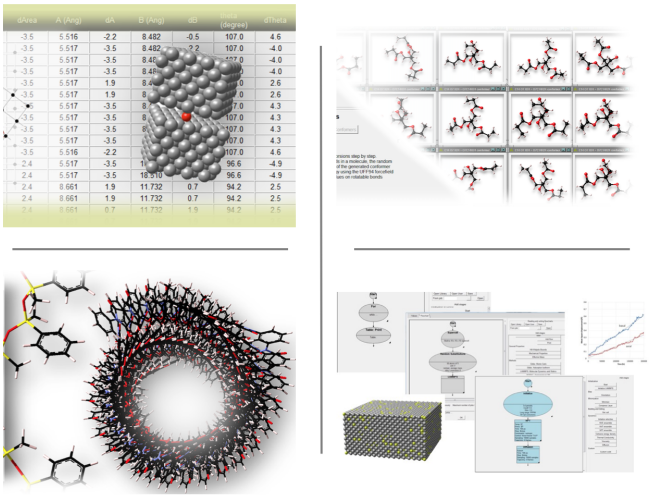
- *MedeA Environment* (Graphical Use Interface): the *main* tier
- *JobServer*: the *middle* tier
- *TaskServer*: the *computational* tier

Users Interact with the *MedeA Environment*, and submit Jobs (i.e. a computational protocols that apply to one or more structures) to the JobServer. A Job can employ multiple simulation runs of specific compute engines, including VASP, LAMMPS, GAUSSIAN, MOPAC, and GIBBS. Each compute engine invocation is called a Task, and will be submitted to computing resources hosting TaskServers.

Platform Support: *MedeA* is a native 64 bit application on both Windows and Linux platforms.

Property Prediction

MedeA's powerful compute engines provide application-specific properties that facilitate sophisticated modeling, analysis, and prediction for materials. These modules work in conjunction with one or more of the compute engines (VASP, GAUSSIAN, MOPAC, GIBBS, and LAMMPS) or use pre-calculated descriptors to obtain or use existing property correlations.



Reproducible Workflows

Benefit from graphical flowcharts in *MedeA* to create and use workflows that combine many stages, each one of which defines a specific operation. To ensure reproducibility and re-usability, flowcharts are stored together with input and output data for reference, can be shared with colleagues, and can form the basis for the development of new procedures.

High-Throughput

High-Throughput tools are available in *MedeA* providing a rich environment for efficient large scale computation, ideal for screening of materials, and exploring material behavior over a range of conditions.

Adapting *MedeA* to Your Needs

Configure your *MedeA Environment* to match your needs. Pick key functionality for your work, and select installation options matching your hardware environment.

Key Features

- *Search and retrieve over 1.1 million entries of materials data, including crystal structure and binary phase diagrams*
- *Explore the vast compositional space of materials efficiently*
- *Build models of solids, surfaces, molecules, nanostructures, and interfaces between materials with a flexible and intuitive user interface*
- *Compute mechanical, thermal, fluid, catalytic, electrical, optical, and magnetic properties of materials*
- *Keep all computed results and data organized with the JobServer*
- *Visualize and analyze results*

Find Out More

Learn more about how *MedeA* can support your work through capabilities such as Databases, Builders, Compute Engines, Forcefields, Property Modules, Analysis Tools, and High-Throughput.

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