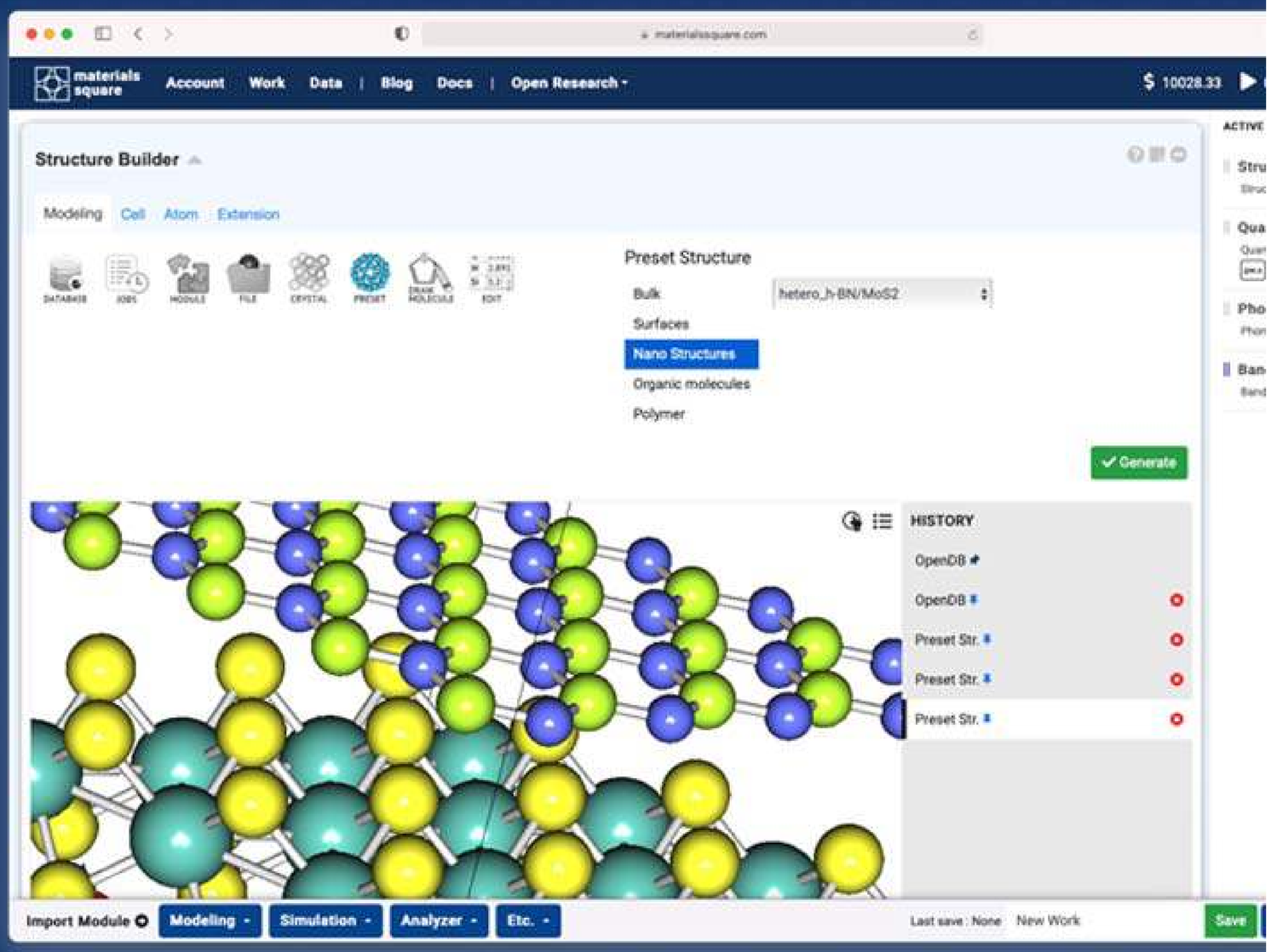
A Cloud-Based Materials Simulation Platform

materials square

matsq.com



Materials Square (**www.matsq.com**) is a cloud-based SaaS platform that facilitates the uptake and execution of materials and molecular atomistic simulations, for the benefit of more efficient R&D innovation and training by academic and industrial researchers alike. For achieving this, the Materials Square web-based simulation platform provides an intuitive graphical user interface, convenient modelling workflows and data management system, and affordable pay-as-you-go access to remote cloud computing providers like AWS. All this is ideally-suited for anyone willing to embrace materials science and chemistry simulations easily. Furthermore, Materials Square offers a user-friendly design for data visualization and analysis, a comprehensive set of machine learning tools, and a powerful 3D atomic structure-builder and modelling interface.

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Cutting-Edge Materials Simulation Techniques

Materials Square provides
strictly verified materials research tools
with intuitive user interfaces
Enjoy high-end simulation/ML tools
without any concerns

Professional Consulting & Technical Support

If you need R&D support,
Materials Square's professional
researcher pool is ready for support

High Performance Computer

Cloud HPCs are provided as
"pay-as-you-go" pricing model.
Improve your R&D cost efficiency
with Materials Square!

Supported Simulation Engines and Techniques

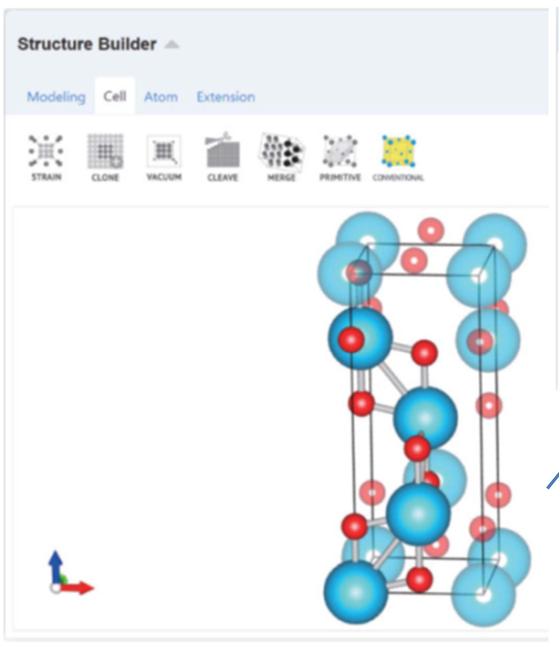
DFT Density Functional Theory — QUANTUMESPRESSO

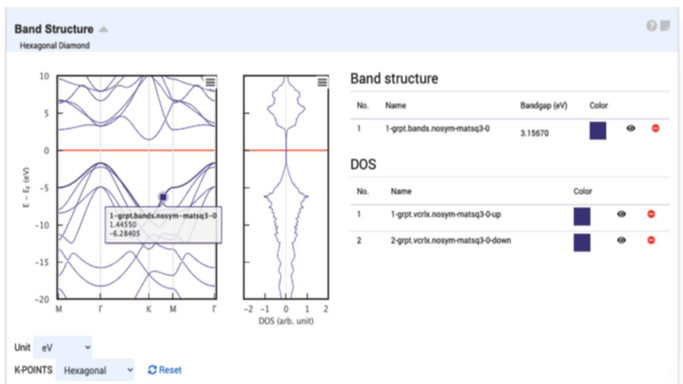
DFT Density Functional Theory — GAMESS

Machine Learning

MD Classical Molecular Dynamics — LAMMPS

OpenCalphad





From the **input structure** to the **output results**, all within the same cloud-powered online platform!

Price (DFT/MD simulation)

PAY-PER-USE: Computing Resources

$0.25 per core hour

Examples of Applications in Industry

Plastic

- Optimization of various compounds
- Biodegradable polymer materials
- Calculation of polymer properties

Alloy Design

- Composition-microstructure relation
- Origin of mechanical properties
- Quantification of microstructural factors

Semiconductor

- Stability of new memory
- Electronic transport behavior
- Current-voltage relation

Solar Cell

- Design highly-efficient solar cell
- Resolve stability and toxicity issue
- Transmittance, absorption coefficient

Catalyst

- Development of organic/inorganic catalyst
- Calculation of catalytic effect
- Refining high efficiency process technology

Battery

- Design next generation battery
- Battery degradation simulation
- Battery charge capacity / Voltage / Speed

Discover also **Katalitic**, our new cloud-based SaaS platform dedicated entirely to the design and discovery of novel catalyst materials!

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Digital Research Cloud for Energy Materials "katalitic"
https://katalitic.io