BIOVIA MATERIALS STUDIO COMPONENT COLLECTION

DATASHEET

The BIOVIA Materials Studio Collection for BIOVIA Pipeline Pilot is a software solution that enables the integration of predictive analytics for materials discovery into automated scientific workflows. Key materials modeling and simulation tools from Materials Studio are supported and integrated with BIOVIA Pipeline Pilot.

The Materials Studio Collection combines the strengths of Materials Studio to predict materials properties, in a wide range of application fields with those of BIOVIA Pipeline Pilot regarding the capture, automation and streamlining of scientific workflows.

In comparison to traditional materials modeling applications, complex workflows can be developed, captured and shared quickly and easily, and protocols executed for large numbers of similar systems. In combination with other BIOVIA Pipeline Pilot collections, workflows can be further enhanced and deployed across the organization.

Use the Materials Studio Collection to Reduce Your Workload and Increase Productivity by:

- Creating multi-step workflows with easy graphical programming
- Automating calculations and deploying essential functions as web-based applications across the enterprise
- Accelerating calculations with new parallel processing options

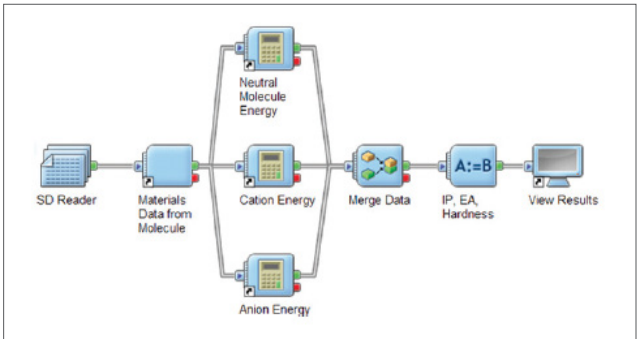

Figure 1: Workflows automate routine calculations, even ones that involve multiple steps. In this example, the ionization potential (IP), electron affinity (EA), and hardness (IP-EA)/2 are computed for a series of structures using Materials Studio DMol^3. Results can be displayed graphically, sorted, and even used as input to subsequent workflows.

HOW DOES THE MATERIALS STUDIO COLLECTION MAKE YOUR JOB EASIER?

Create Multi-Step Workflows

Some properties require multiple calculations with different programs to yield the needed result. For example, constructing an amorphous polymer requires many steps including building the monomer units, packing a unit cell, equilibrating the result, and taking ensemble averages. Users can benefit tremendously by automating these processes. The Materials Studio Collection makes it easy for even first-time users to create sophisticated workflows that save time and simplify modeling tasks.

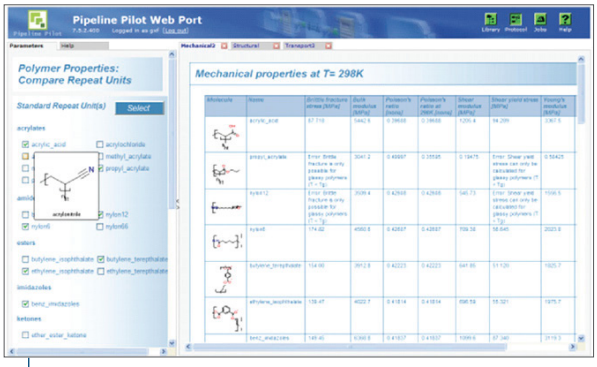

Figure 2: The Materials Studio Collection lets you create web portals to deploy key functions enterprise-wide. In this example, the Polymer Properties components have been used to provide a tool with which a wide range of users can select or enter structures and request properties. Results are displayed in tabular form for easy viewing and sharing.

Automate and Deploy Functions Enterprise-Wide

Many researchers need to compute the same properties over and over. Heats of formation, band gaps, elastic constants, vibrational spectra, and solubility parameters are among the many types of calculations that can be automated with the Materials Studio Collection. Automation eliminates human error and relieves the tedium of such calculations. With the click of a button, compute the properties you need for a long list of compounds and then see the results presented in a customizable report. In combination with BIOVIA Pipeline Pilot Web Port, you can also deploy these calculations to other colleagues in your organization through simple web-based interfaces.

Accelerate Calculations with New Parallel Processing Options

Whether you are simply changing input parameters such as pressure, exploring a vast number of material compositions, or running many calculations for good statistical averaging, materials discovery or optimization often involves multiple calculations. Using the Materials Studio Collection for BIOVIA Pipeline Pilot enables you to run calculations using both a coarse- and fine-grained approach. BIOVIA Pipeline Pilot can distribute your work across compute servers, clusters and cores to optimize the use of your computational resources, dramatically reducing your time to solution.

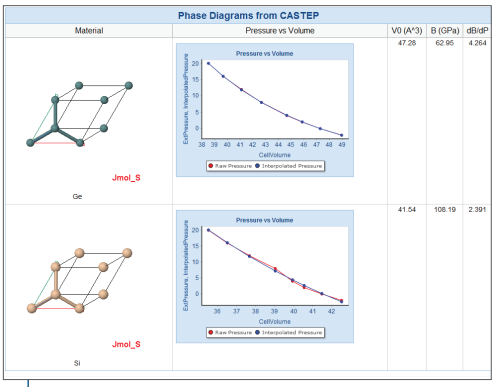

Figure 3: Predictive analytics on whole series of compounds becomes simple, as structures can be read in from different data sources and properties determined within one protocol. The calculations are run in a coarse-grained parallel approach so each calculation is submitted to its own server. The results are automatically collated from the separate jobs for reporting.

ABOUT THE MATERIALS STUDIO COLLECTION FOR BIOVIA PIPELINE PILOT

The Materials Studio Collection:

- Allows Materials Studio applications to be used within a drag-and-drop workflow management environment
- Includes a range of property calculators and enables complex properties to be encapsulated easily by constructing protocols
- Provides viewing and reporting capabilities as well as easy interoperability with Materials Studio
- Enables high-throughput computation through seamless integration with BIOVIA Pipeline Pilot, streamlining materials discovery and optimization

THE MATERIALS STUDIO COLLECTION INCLUDES:

Classical Simulations Components

Construct amorphous models of small molecules and polymers, pack molecules into existing structures, and build layered structures with components based on Materials Studio Amorphous Cell. After construction, geometry optimization and molecular dynamics components based on Materials Studio Forcite Plus enable equilibration and production runs of time dependent properties. Key properties such as the cohesive energy density, solubility parameter, viscosity, and elastic constants can be calculated.

Quantum Mechanics Components

Use the accurate density functional quantum mechanics modules, Materials Studio NMR CASTEP and Materials Studio DMol^3, to calculate energies, optimize geometries, and run molecular dynamics of molecules and crystals. Predict a wide variety of properties including reactivity indices, band structures, density of states, and other electronic properties. The fast semi-empirical Materials Studio VAMP module enables screening of thousands of compounds calculating properties such as dipole moments, atomic polarizabilities, spectra, orbital energies and solvent effects.

Analysis Components

Perform basic analysis to examine geometrical properties such as angle, distance, and torsion distribution. Calculate structural properties such as radial distribution function and radius of gyration.

Readers, Writers and Convertor Components

Read in common structural formats such as CIF, multiframe trajectories, and study tables. Write out native Materials Studio structures and study tables. Convert between Materials and Chemistry objects to harness functionality from other collections.

Crystallization Components

Use the Polymorph components to build customized polymorph prediction workflows. Use the BIOVIA Pipeline Pilot environment to enable coarse grained parallelization, allowing you to submit each space group to a separate CPU. Use the Reflex components to create simple workflows for manipulating powder diffraction data, or automate complex tasks such as structure solution. Use example protocols to validate crystal structures or match powder patterns to structures.

Manipulator Components

Read in a series of molecules and automatically add hydrogens and perform an initial clean of the geometry. Build crystals, surfaces and layered structures, enabling full manipulation of the symmetry of the system. Cleave surfaces from crystal structures. Read in trajectories and create subsets, new trajectories, and split original trajectories.

Property Calculator Components

Calculate simple properties such as 2D or 3D periodicity of the system and associated lattice information, molecular weight of a molecule, or charge on an atom. Couple Materials Studio QSAR descriptors such as Chi and Kappa indices with the powerful model building tools in the BIOVIA Pipeline Pilot Data Modeling & Statistics to build structure-property models.

MaterialsScript Components

Harness the full power of MaterialsScript by creating customized components that you can drag and drop into other workflows or deploy to your customers. Extend the properties that you can calculate and add to the pipeline.

Polymer Property Components

Quick and easy generation of polymer properties based on the most recent edition of Bicerano's popular "Prediction of Polymer Properties" book.[1] Estimate properties such as glass transition, thermal conductivity, and interfacial tension.

Viewer and Reporting Components

Use the Jmol viewer to visualize molecular and crystal structures, including incorporation of symmetry in the view. View static images, rotatable models, and animatable trajectories and embed them in webpages and other documents.

ADVANCED PROPERTY PREDICTION

Through job automation and integration with pipeline pilot components, advance materials property calculations can be executed using advanced, fully configured protocols. Those provided include

Polymers

- A protocol for creating polymer network structures using a multistep reaction mechanism
- Calculation and analysis of glass transition temperature
- Calculation of yield stress and critical distortional strain

These protocols post-process raw data with automatic curve fitting procedures and provide detailed summary reports to streamline property prediction simulations.

Metal Alloys

- Composition dependent bulk mechanical and thermal property prediction using a cluster expansion methodology
- Composition dependent bulk mechanical and thermal property prediction using a quasi-random structure approach
- Thermal conductivity via Kubo-Greenwood formula applied to molecular dynamics trajectories
- Temperature dependent mechanical properties of metals using phonon free energy evaluations at various fixed cell volumes

ABOUT BIOVIA PIPELINE PILOT

BIOVIA Pipeline Pilot is an enterprise-scalable scientific informatics platform that enhances research and development organizations' ability to innovate by uncovering scientific value locked in disparate data silos, automating scientific workflows, and facilitating collaboration throughout the wider scientific community. BIOVIA Pipeline Pilot's Component Collections are the "scientific building blocks" of the platform and are grouped by category of science or function. By graphically combining components, you can construct workflows for data retrieval, filtering, analysis, and reporting.

To learn more about BIOVIA Materials Studio, go to **3dsbiovia.com**/materials-studio

REFERENCES

1. J. Bicerano, Prediction of Polymer Properties, Marcel Dekker, Inc., New York, 2002.

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