DASSAULT SYSTEMES

BIOVIA

WHAT'S NEW IN BIOVIA MATERIALS STUDIO 2017 R2

DATASHEET

BIOVIA Materials Studio 2017 R2 is the latest release of BIOVIA's predictive science tools for researchers in materials science and chemistry. Materials Studio empowers researchers to understand the relationships between a material's atomic and molecular structure and its properties.

Using Materials Studio 2017 R2, scientists can model and evaluate the structure-property relationships of many materials types to shorten product innovation lifecycles. In addition, now chemists and chemical engineers may bring together the power of quantum mechanics and reaction kinetics models to predict chemical reactions in realistic reaction vessel and combustion simulations.

MORE SCIENCE

New module for reaction kinetics

Exposure of the highly regarded Cantera [www.cantera.org] chemical kinetics simulation package though Materials Studio Visualizer enables scientists to seamlessly combine experimental and quantum mechanically derived reaction rate data and then predict reactant/product concentrations in various reactor environments.

MORE MATERIALS

CASTEP OTFG norm-conserving potentials now cover the whole periodic table and additional parameters for DFTB+ and GULP increase further the range of materials accessible to simulation.

MORE PROPERTIES

Workflow automation in Pipeline Pilot allows efficient, convenient access to advanced computation and analysis. Protocols are now available for bulk polymers properties (including network building routines) and metal and metal alloy property predictions.

MATERIALS STUDIO 2017 R2 HIGHLIGHTS

A new module Materials Studio Cantera!

- New feature! Cantera Reaction editor enables users to introduce new species and reactions into complex reaction schemes whilst keeping the data thermodynamically consistent.
- New feature! Gas phase reactions at equilibrium, in continuous stirred reactors, and in 1D Flame models.

Quantum Mechanics Highlights

- New properties! EPR G-Tensor predictions from CASTEP, Empirical Hardness models from CASTEP and DMol3, and solvation free energies from ONETEP.
- Enhanced performance! Much faster CASTEP Raman for large models.
- Improved accuracy! OTFG norm-conserving potentials for rare-earth 4f/5f elements.
- More materials! New DFTB+ libraries for electronic structure of Si, SiO2 and their interfaces plus new smearing options to converge difficult cases.
- New properties! New DFTB+ Mechanical Properties Task
- Enhanced usability! Availability of partial Hessians for CASTEP, DMol3 and DFTB+ models.

Visualization and Collaboration Highlights

- Enhanced usability! Custom formatting of job folder names and support of non-native files within the MS project.
- Enhanced usability! Clean molecules within periodic structures and use new controls for object visibility in 3D models.

Workflow Automation Highlights (via Pipeline Pilot Materials Studio Collection)

- New Protocols! For building chemically crosslinked 3D-polymer models, calculating glass transition and yield stress all from sketched monomer input models.
- New Protocol! Implementing cluster expansion method for metal alloy property prediction.
- New Protocol! Calculate temperature dependent mechanical properties using CASTEP.

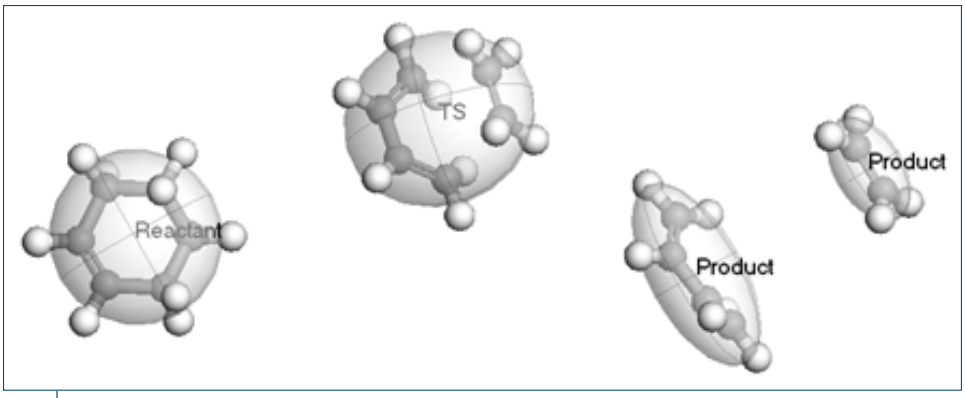

Figure 1: Transition states derived from quantum mechanics calculations provide the reaction barriers for reaction pathways for the cases where they are otherwise unavailable.

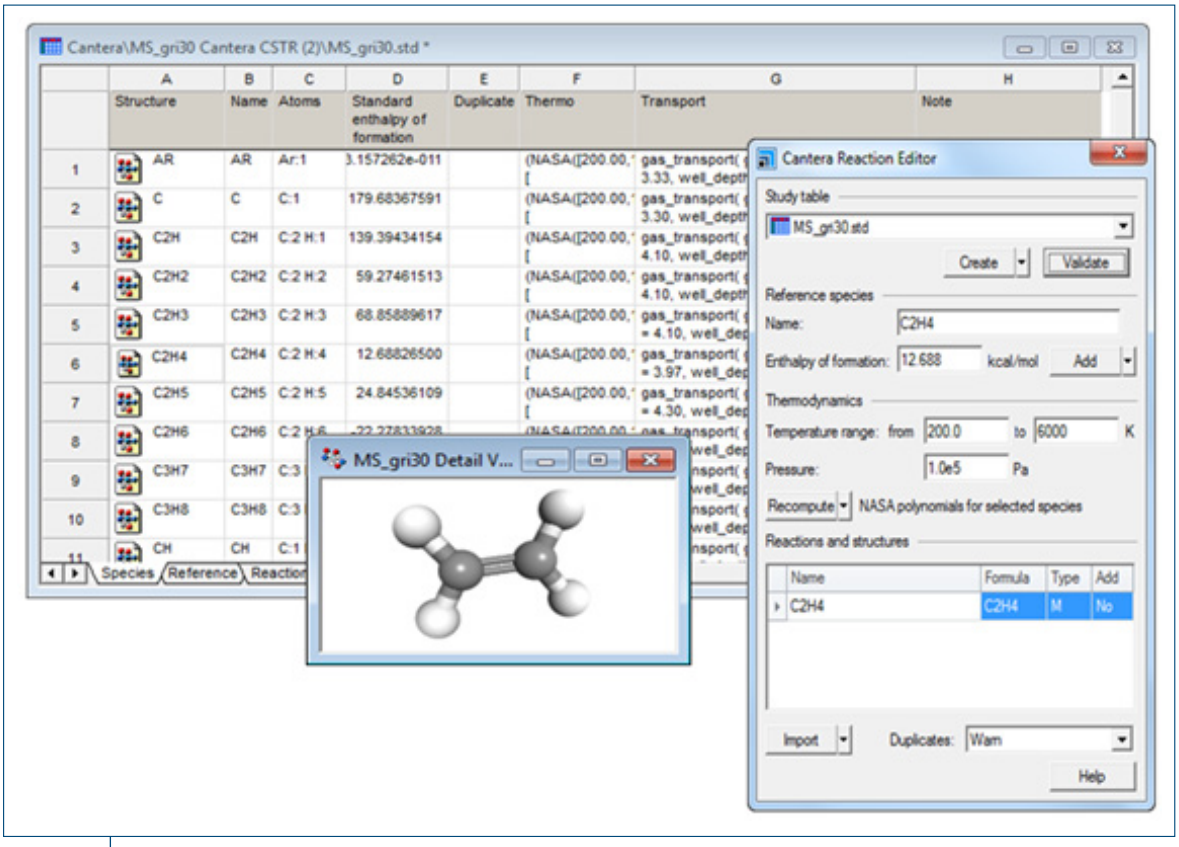

Figure 2. Materials Studio provides a unified environment for collating, verifying input and executing Cantera calculations.

Our **3D**EXPERIENCE Platform powers our brand applications, serving 12 industries, and provides a rich portfolio of industry solution experiences.

Dassault Systèmes, the **3D**EXPERIENCE Company, provides business and people with virtual universes to imagine sustainable innovations. Its world-leading solutions transform the way products are designed, produced, and supported. Dassault Systèmes' collaborative solutions foster social innovation, expanding possibilities for the virtual world to improve the real world. The group brings value to over 170,000 customers of all sizes in all industries in more than 140 countries. For more information, visit **www.3ds.com**.

3DEXPERIENCE®

DASSAULT SYSTEMES | The **3D**EXPERIENCE® Company

Dassault Systèmes Corporate
Dassault Systèmes
175 Wyman Street
Waltham, Massachusetts
02451-1223
USA

BIOVIA Corporate Americas
BIOVIA
5005 Wateridge Vista Drive,
San Diego, CA
92121
USA

BIOVIA Corporate Europe
BIOVIA
334 Cambridge Science Park,
Cambridge CB4 0WN
England