BIOVIA Materials Studio

2016 Training Course Catalog

3DEXPERIENCE®

Contents

SUMMARY

We are proud to offer a variety of courses to meet your organization's needs. Customized courses can be designed to meet your organization's specific needs, please contact your Account Manager.

Delivery Methods:

- Instructor-Led Training (ILT): Facilitated by an onsite instructor, this training takes place at your location or at a selected Biovia site. Onsite courses offer hands-on exercises to enhance the learning experience.
- Web-Based Training: Our instructors teach these courses virtually allowing students to attend from their remote location. Hands-on exercises are assigned as homework in these web-based classes.

INSTRUCTOR-LED COURSES

Introduction to Materials Studio

This workshop provides an introduction to the tools and functionality available in Materials Visualizer, the core modules in the Materials Studio suite of software.

Topics	Details
• Materials Studio – Interface and sketching – Builders: polymer, crystal, nano, meso – Tools • Materials Modeling – Multiscale, quantum, MM, meso, Crystal, QSAR • Scripting in Materials Studio • Using the client-server architecture • Problem-solving approaches	**Onsite Duration**: 1 Day **Web-Based Duration**: 3 Hours **Prerequisites**: None

Adsorption Locator

BIOVIA Materials Studio Adsorption Locator helps you to find the most stable adsorption sites for a broad range of materials, including zeolites, carbon nanotubes, silica gel, and activated carbon – to name just a few, by carrying out Monte Carlo searches of the configurational space of the substrate-adsorbate system.

Topics	Details
• Theory in Adsorption Locator • Computational Tasks in Adsorption Locator • Results from Adsorption Locator • Scripting • Comparison with Sorption	**Onsite Duration**: 2 Hours **Web-Based Duration**: 1 Hour **Prerequisites**: Introduction to Materials Studio

Amorphous Cell

BIOVIA Materials Studio Amorphous Cell is a comprehensive model building tool for creating a wide range of amorphous materials. The behavior of amorphous materials is critical to products such as plastics, glasses, foods, and chemicals.

Topics	Details
• Introduction • The Construction Task • How It Works • The Packing and Confined Layer Tasks • Scripting with Amorphous Cell • Tips and Case Studies	**Onsite Duration:** 0.5 Day **Web-Based Duration:** 1 Hour **Prerequisites**: Introduction to Materials Studio

Blends

BIOVIA Materials Studio Blends is used to predict phase diagrams and interaction parameters for liquid-liquid, polymer-polymer, and polymer-additive mixtures in order to study the structural factors affecting the behavior of blends and formulations.

Topics	Details
• Theory in Blends • Tasks and Analysis in Blends • Phase Diagrams • Applications and Limitations	**Onsite Duration**: 2 Hours **Web-Based Duration**: 1 Hour **Prerequisites**: Introduction to Materials Studio

CASTEP, Introduction

BIOVIA Materials Studio CASTEP is an ab initio quantum mechanical program employing Density Functional Theory (DFT) to simulate the properties of solids, interfaces, and surfaces for a wide range of materials classes such as ceramics, semiconductors, and metals. First principle calculations allow researchers to investigate the nature and origin of the electronic, optical, and structural properties of a system without the need for any experimental input.

Topics	Details
• Introduction to Solid-State Theory and Density Functional Theory (DFT) • Technical aspects of DFT calculations • Computational tasks in CASTEP • Chemical reactions with CASTEP: Transition state search • Properties calculations in CASTEP	**Onsite Duration**: 0.5 Day **Web-Based Duration**: 3 Hours **Prerequisites**: Introduction to Materials Studio

CASTEP, Advanced

The CASTEP advanced course offers detailed introduction to accurate prediction of electronic properties, NMR, STM, phonon spectra, core-level spectra, and optical properties.

Topics	Details
• Introduction • Electronic Properties – Band structure – Density of states – Electron density difference – Wave Functions – Fermi surfaces • Experimental Properties – NMR – STM – Phonons, IR and Raman spectroscopy – Optical Spectroscopy – Core-level Spectroscopy – Work Function	**Onsite Duration**: 0.5 Day **Web-Based Duration**: 3 Hours **Prerequisites**: • Introduction to Materials Studio • CASTEP, Introduction

Conformers

BIOVIA Materials Studio Conformers provides access to a comprehensive collection of conformational searching and analysis techniques to characterize molecular conformation and flexibility, to gain insight into geometric and energetic properties, and to probe geometry-property relationships, which have application in many fields including crystallization, catalysis, and polymer studies.

Topics	Details
• Conformers Search Methods – Systematic Grid Scan – Random Sampling Search – Boltzmann Jump Search • Calculation Setting Up and Output – Preparing the Structure – Conformers Calculation – Filter – Output	**Onsite Duration**: 2 Hours **Web-Based Duration**: 1 Hour **Prerequisites**: Introduction to Materials Studio

DFTB+

BIOVIA Materials Studio DFTB+ is an improved implementation of the Density Functional-based Tight Binding (DFTB) quantum simulation method for the study of electronic properties of materials. DFTB+ offers unique capabilities to study and understand systems containing hundreds of atoms. Problems that took more time or compute power than most researchers have available, such as defects in semi-conductors, and interactions between organic and inorganic surfaces, are now practical to study using DFTB+.

Topics	Details
• Introduction to DFTB+ • Derivation of the DFTB+ Method • Computational Tasks in DFTB+ • Properties Calculation • Creating Slater-Koster Parameters with the Parameterization Tool • Electron Transport Calculations • Case Studies	**Online Duration**: 1 Day **Web-Based Duration**: 3 Hours **Prerequisites**: Introduction to Materials Studio

DMol^3, Introduction

BIOVIA Materials Studio DMoL^3 combines computational speed with the accuracy of quantum mechanical methods to predict materials properties reliably and quickly. It can predict processes in gas phase, solution, and solid environments. It is broadly applicable to research problems in chemistry, pharmaceuticals, materials science, and chemical engineering, as well as solid state physics.

Topics	Details
• Introduction To Solid State Theory and Density Functional Theory (DFT) • Technical Aspects Of DFT Calculations • Computational Tasks In Dmol^3 • Properties Calculations In Dmol^3	**Onsite Duration**: 0.5 Day **Web-Based Duration**: 3 Hours **Prerequisites**: Introduction to Materials Studio

DMol^3, Advanced

The DMol^3 advanced course offers detailed introduction to accurate prediction of electronic properties, chemical reactions, IR and Raman spectra, optical properties, and electron transport properties.

Topics	Details
• Properties calculations in DMol3 – Band structure – Density of states (DOS) – Electron densities – Electrostatics – Molecular orbitals – Atomic populations • Experimental Properties – Chemical reactions – Vibrations and vibration spectroscopy – Optical excitations and optical spectroscopy – Electron transport	**Onsite Duration**: 0.5 Day **Web-based Duration**: 3 Hours **Prerequisites**: • Introduction to Materials Studio • DMol^3, Introduction

Forcite and Forcite+

BIOVIA Materials Studio Forcite is an advanced classical molecular mechanics tool that allows fast energy calculations and reliable geometry optimization of molecules and periodic systems. Forcite provides the user with great flexibility, offering a range of forcefields and charging methods.

Topics	Details
• Introduction to Forcefield – Forcefield types – Nonbond interactions – Forcefield typing and change assignment • Computational tasks in Forcite • Forcefield analysis • Forcefield editing • Scripting in Forcite	**Onsite Duration**: 1 Day **Web-Based Duration**:3 Hours **Prerequisites**: Introduction to Materials Studio

GULP

The General Utility Lattice Program, or BIOVIA Materials Studio GULP, is a classical simulations code for performing a wide range of calculations on 3D periodic solids, 2D surfaces, gas phase clusters, and isolated defects in a bulk material. In particular, GULP has a large number of materials-specific forcefields, such as the shell model for simulating ionic materials.

Topics	Details
• Theory in GULP • Computational Tasks in GULP • Forcefield Fitting • Surface Properties • Properties Calculation • Applications	**Onsite duration**: 1 Day **Web-Based Duration**: 3 Hours **Prerequisites**: Introduction to Materials Studio

Materials Studio Collection in Pipeline Pilot (MSC in PP)

The BIOVIA Pipeline Pilot Materials Studio is a new software solution that allows access and utilization of Materials Studio's premier modeling capabilities within the Pipeline Pilot™ scientific authoring application. Now you can integrate predictive analytics for materials properties seamlessly into your scientific workflows. This allows for a more streamlined approach to materials discovery and improves productivity so that you can spend more time on innovation and less on costly laboratory experimentation.

Topics	Details
• Readers, Writers, Viewer, and Reporting Components • Manipulation • Property Calculators • Quantum Mechanics • Classical Simulation • Crystallization • Using the Materials Toolkit • The Pipeline Pilot Connector for Materials Studio • Parallel Processing	**Onsite Duration:** 1 Day **Web-Based Duration**: 3 Hours **Prerequisites**: Introduction to Materials Studio

Mesodyn

MesoDyn is a dynamic simulation method for studying the long length and time behavior of complex fluid systems, including polymer melts and blends. MesoDyn takes a coarse-grained description of a complex fluid and performs time-evolution dynamics of the density and potential fields of the system.

Topics	Details
• Introduction to Mesoscale Simulations • Density Functional Theory in MesoDyn • Set Up of MesoDyn Calculations • Analysis of MesoDyn Calculations • Applications	**Onsite Duration:** 0.5 Day **Web-Based Duration**: 2 Hours **Prerequisites**: Introduction to Materials Studio

Mesocite (DPD)

BIOVIA Materials Studio Mesocite is a state-of-the-art coarse-grained simulation module for the study of materials at length scales ranging from nanometers to micrometers and time scale from nanoseconds to microseconds. Such materials pervade industrial research in areas such as composites, coatings, cosmetics, and controlled release. Mesocite can provide structural and dynamic properties of fluids in equilibrium, under shear or in confined geometries

Topics	Details
• Introduction to Mesocite • Building Meso-Structures • Introduction to Dissipative Particle Dynamics • Mesoscale Parameter Generation (DPD) • Mesocite DPD Setup • Mesocite Task Setup • Mesocite Analysis & Scripting	**Onsite Duration:** 0.5 Day **Web-Based Duration:** 2 Hours **Prerequisites**: Introduction to Materials Studio

Morphology

BIOVIA Materials Studio Morphology allows you to predict crystal morphology from the atomic structure of a crystal. The application areas include pharmaceuticals, agrochemicals, food sciences, petrochemicals, cements, and commodity and specialty chemicals.

Topics	Details

• Theory in Morphology
  – Predicting Morphologies
  • Bravais-Friedel Donnay-Harker (BFDH) method
  • Growth morphology method
  • Equilibrium morphology method
  – Crystal Graphs
• Tasks and Analysis in Morphology
• Problems in Surface Chemistry
	Onsite Duration: 2 Hours
	Web-Based Duration: 1 Hour
	Prerequisites: Introduction to Materials Studio

ONETEP

BIOVIA Materials Studio ONETEP is a linear scaling method, meaning the time required for a calculation increases linearly with the number of atoms. This linear scaling approach is a vast improvement over conventional DFT methods, where the time needed for computation increases at a rate of as much as N3 (where N is the total number of atoms). As a result, the program can be used to model systems larger than possible by using conventional DFT.

Topics	Details
• ONETEP Theory • Setup of ONETEP Calculations • ONETEP Properties and Analysis • Case Studies	**Onsite Duration**: 1 Day **Web-Based Duration**: 3 Hours **Prerequisites**: Introduction to Materials Studio

Polymorph

BIOVIA Materials Studio Polymorph is used to predict potential polymorphs of a given compound directly from the molecular structure. It explores and ranks polymorphs of fairly rigid, non-ionic or ionic molecules. The approach is based on the generation of possible packing arrangements in all reasonable space groups to search for the low lying minima in lattice energy.

Topics	Details
• Determination of Crystal Structures • Theory Behind Polymorph Prediction • Setting Up Polymorph Calculations • Analyzing the Results • Scripting with the Polymorph Module • Applications	**Onsite Duration**: 0.5 Day **Web-Based Duration**: 1 Hour **Prerequisites**: Introduction to Materials Studio

QMERA

The BIOVIA Materials Studio QMERA module in BIOVIA Materials Studio performs simulations by combining DFT methods from DMol^3 and force field methods from GULP. QMERA can be used to model either molecular or periodic systems and can handle hundreds or even thousands of atoms. It is particularly well-suited for modeling problems in chemical reactivity, where an active site is chemically localized. Researchers can use the method to study problems in nanotubes, nanoclusters, and amorphous material.

Topics	Details
• Overview of QM/MM • The QM/MM Embedding Schemes • Handling of the QM/MM Boundary • General Consideration for Simulations • QMERA Tasks & Analysis • QMERA Servers: DMol^3 and GULP • Applications	**Onsite Duration**: 1 Day **Web-Based Duration**: 3 Hours **Prerequisites**: Introduction to Materials Studio

QSAR

The QSAR module is a comprehensive set of tools for creating statistical regression models between experimental information ('activity') and molecular level characteristics ('descriptors'). The descriptors that can be calculated include a wide range of properties. These can be supplemented by characteristics calculable with other modules: Forcite, VAMP, fast descriptors.

Topics	Details
• Introduction to QSAR • Initial Data Analysis • Descriptors • Model Building • Genetic Function Approximation • Model Validation and Prediction	**Onsite Duration**: 1 Day **Web-Based Duration:** 3 Hours **Prerequisites**: Introduction to Materials Studio

Reflex, Reflex-Plus, X-Cell, and Reflex QPA

BIOVIA Materials Studio Reflex simulates X-ray, neutron, and electron powder diffraction patterns based on models of crystalline materials. Reflex aids the determination of crystal structure, assists the interpretation of diffraction data, and is applied to validate the results of experiment and computation.

Topics	Details
• Introduction to Reflex Tools • Pattern Processing Tool • Powder Indexing Tool • Powder Refinement Tool • Powder Solve Tool - Separately licensed modules • Powder QPA (Quantitative Phase Analysis) Tool - Separately licensed modules • Powder Crystallinity Tool	**Onsite Duration**: 1 day **Web-Based Duration**: 3 Hours **Prerequisites**: Introduction to Materials Studio

Scripting in Materials Studio

This workshop provides an introduction into the Perl-based scripting language that allows access to some of the Visualizer Tools, the Properties Explorer, a range of 3D Atomistic Documents, Study Tables and the Forcite Module (Calculations and Analysis). Students write scripts to draw molecules from scratch; to get information from collection documents, information from trajectory documents, information from study tables; to move molecules (in a zeolite and over a surface), to set up Forcite calculations, and to retrieve selected results along with additional examples

Topics	Details
• Introduction to Scripting in Materials Studio • Scripting for Documents • Scripting for Tools • Scripting for Modules	**Onsite Duration**: 1 Day **Web-Based Duration**: 3 Hours **Prerequisites**: Introduction to Materials Studio

Sorption

Molecular adsorption into microporous structures such as zeolites, aluminophosphates, or polymers is crucial in numerous applications including air separation, hydrocarbon cracking, gas sensors, and ion exchange. BIOVIA Materials Studio Sorption provides a means of predicting fundamental properties, such as sorption isotherms (or loading curves) and Henry's constants, needed for investigating separations phenomena. In addition, modeling can be used to rationalize sorption properties in terms of molecular level processes.

Topics	Details
• Tasks – Fixed Pressure – Fixed Loading – Henry Constant – Adsorption Isotherm – Sorbate Location • Configuration Sampling – Monte Carlo Methods • Other DialogTabs: – Energy – Constraints – Properties • Simulation Tips • Scripting • Adsorption Locator vs. Sorption	**Onsite Duration:** 2 Hours **Web-Based Duration:** 1 Hour **Prerequisites**: Introduction to Materials Studio

Synthia

BIOVIA Materials Studio Synthia calculates polymer properties using advanced Quantitative Structure-Property Relationships (QSPRs). It allows researchers to rapidly screen candidate polymers for a wide range of properties, and allows the property prediction of copolymer blends.

Topics	Details
• Introduction • Quantitative Structure Property Relationship (QSPR) • Synthia - Connectivity Indices Methods • Random Copolymers • Simulation Tips	**Onsite Duration**: 2 Hours **Web-Based Duration**: 1 Hour **Prerequisites**: Introduction to Materials Studio

VAMP

BIOVIA Materials Studio VAMP is a semi-empirical molecular orbital package for molecular organic and inorganic systems. VAMP is an ideal intermediate module between forcefield and first principles methods and is capable of rapidly calculating many physical and chemical molecular properties.

Topics	Details
• Theory in VAMP – NDDO: MNDO/C, MNDO, AM1, PM3, AM1*, MNDO/d, and PM6 – ZINDO: CNDO/1, CNDO/2, INDO/1, and INDO/2 • Calculation Setting Up • Properties Calculations and Analysis • Case Study – Carbon Nanodots (CNDs): Supramolecular Electron Donor–Acceptor Hybrids Featuring Perylenediimides	**Onsite Duration**: 2 Hours **Web-Based Duration**: 1 Hour **Prerequisites**: Introduction to Materials Studio