Materials Studio Official Training by Accelrys

Monday 2nd

Introduction to Materials Studio

This workshop provides an introduction to the tools and functionality available in materials Visualizer, the core module in the Materials Studio suite of software. It is available both on-site and on-line:

- **Managing projects using the Project Explorer.**
- **Sketching simple molecules.**
- **Sketching complex molecules such organometallics using the fragment sketcher.**
- **Defining fragments and repeat units to build polymers.**
- **Analyzing and adjusting geometrical properties such as torsions, angles and distances.**
- **Using the symmetry tools for molecular and periodic systems.**
- **Working with the different display style options.**
- **Integration with publishing software.**
- **Building crystals and surfaces.**
- **Building layered structures and crystal interfaces.**
- **Working with volumetric data - isosurfaces and slices.**

Tuesday 3rd

DMol3

- **Basic concepts on molecular modeling (internal coordinates, numerical basis sets, core treatment, exchange-correlation potentials, smearing)**
- **Solvent effects**
- **Basic concepts in solid state modeling (bands, slabs, gaps, reciprocal space, periodic boundary conditions, Bloch's theorem)**
- **SCF**
- **Tasks (energy, geometry optimisation, dynamics, transition states)**
- **Properties (band structures, density of states (DOS), electron density, electrostatics, frequency à thermodynamic properties, Fukui functions, orbitals, population analysis)**

CASTEP

- **Basic concepts in solid state modelling (bands, slabs, gaps, reciprocal space, Brillouin zone, plane waves, periodic boundary conditions, Bloch's theorem, exchange-correlation potentials, cut-off energies)**
- **SCF**
- **Smearing**
- **Tasks (energy, geometry optimisation, dynamics, elastic constants, transition states)**
- **Properties (band structure, density of states, electron density difference, NMR, optical properties, phonon dispersion, phonon density of states, electric field response, population analysis, stress, thermodynamic properties)**

Wednesday 4th

VAMP

- **Semiempirical Methods**
- **Tasks (Energy, geometry optimization, transition states)**
- **Configuration Interaction**
- **Solvent Effects**
- **Properties (thermodynamics, localized orbitals, IR and Raman spectra, absorption spectra, heats of formation, ionization potentials, bond orders, Mulliken and Coulson charges, polarizabilities, 13C shifts, fluorescence data)**

Amorphous Cell

- **Periodic Boundary Conditions**
- **How the amorphous cell is constructed**
- **Some tips how to handle difficult cases, e.g. stiff polymer chains**
- **Protocols**
- **Analysis (pair correlation function, scattering curve)**

Forcite +

- **Concept of Molecular Modeling**
- **Forcefields (first order second order, rule-based)**
- **Non-bonded interactions**
- **Cut-offs (atom based, group based, Ewald)**
- **Minimisation algorithm**
- **Molecular dynamics**
- **Ensembles**
- **How to analyse trajectories**
- **How to interpret the results**

Thursday 5th

Mesodyn & DPD

- **Concept of Mesoscale Modeling**
- **The Gaussian Chain**
- **DPD Theory**
- **MesoDyn Theory**
- **How to get Mesoscale Parameters**
- **Analysing the results**
- **Visualizing the results**
- **Building mesostructures using the mesostructure template dialog**

Friday 6th

Scripting in Materials Studio

- **Understanding of principles of the scripting language.**
- **How to work with the scripting editor and how to apply it to**
  - **Atomistic Documents (.xsd)**
  - **Collection Documents (.xod)**
  - **Trajectory Documents (.xtd)**
  - **Study Tables (.std)**
  - **Tools**
  - **Forcite**
  - **DMol**
  - **Reflex Tool**
- **Writing scripts to draw molecules from scratch, to get information from collection documents, to get information from trajectory documents, to get information from study tables, to move molecules (in a zeolite and over a surface), to set up Forcite calculations and retrieve selected results and some more examples**

Introduction to Materials Studio Collection in Pipeline Pilot

End of the training

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