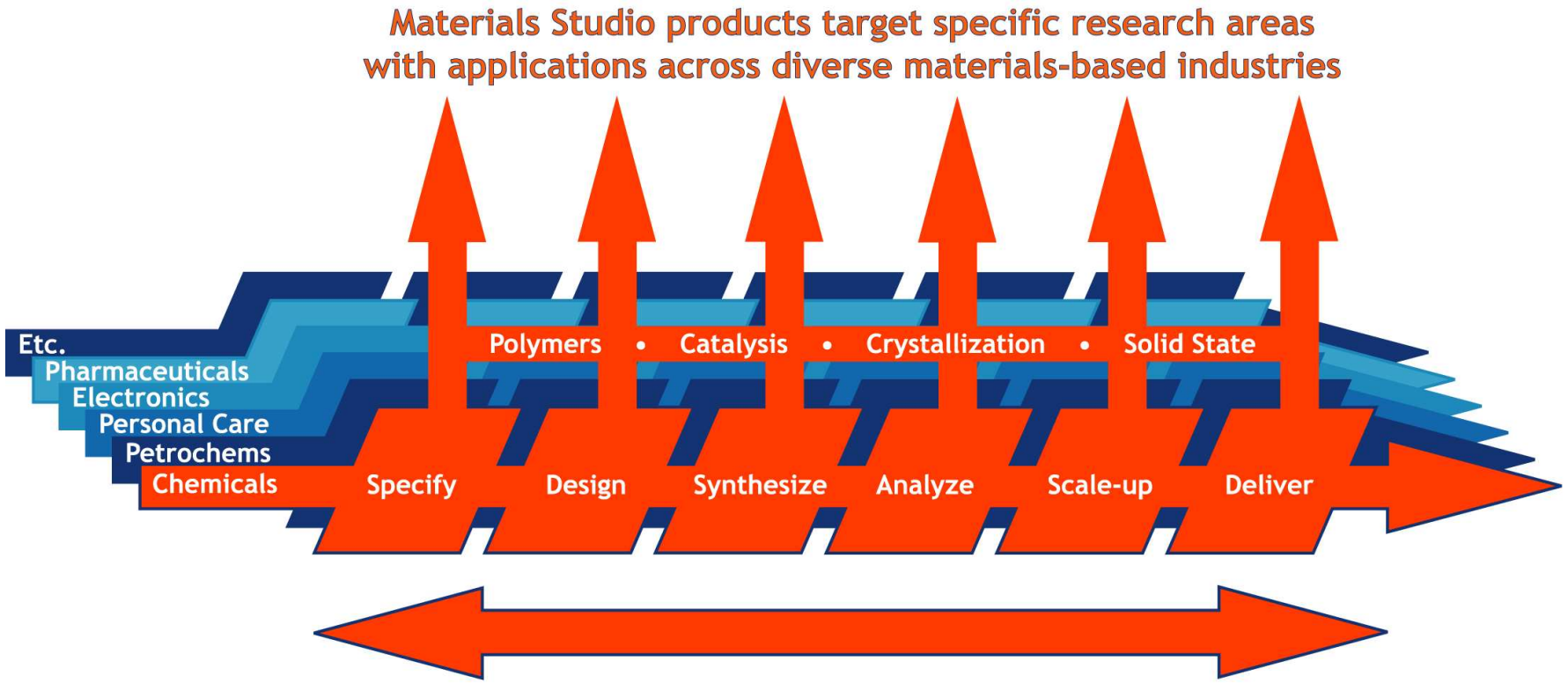
Introducing Materials Studio



MATERIALS STUDIO

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MS Modeling

Expert-level modeling and simulation for materials research in an easy-to-learn yet powerful PC-based environment

MS Matinformatics

Data, information, and knowledge management for the chemical process industries

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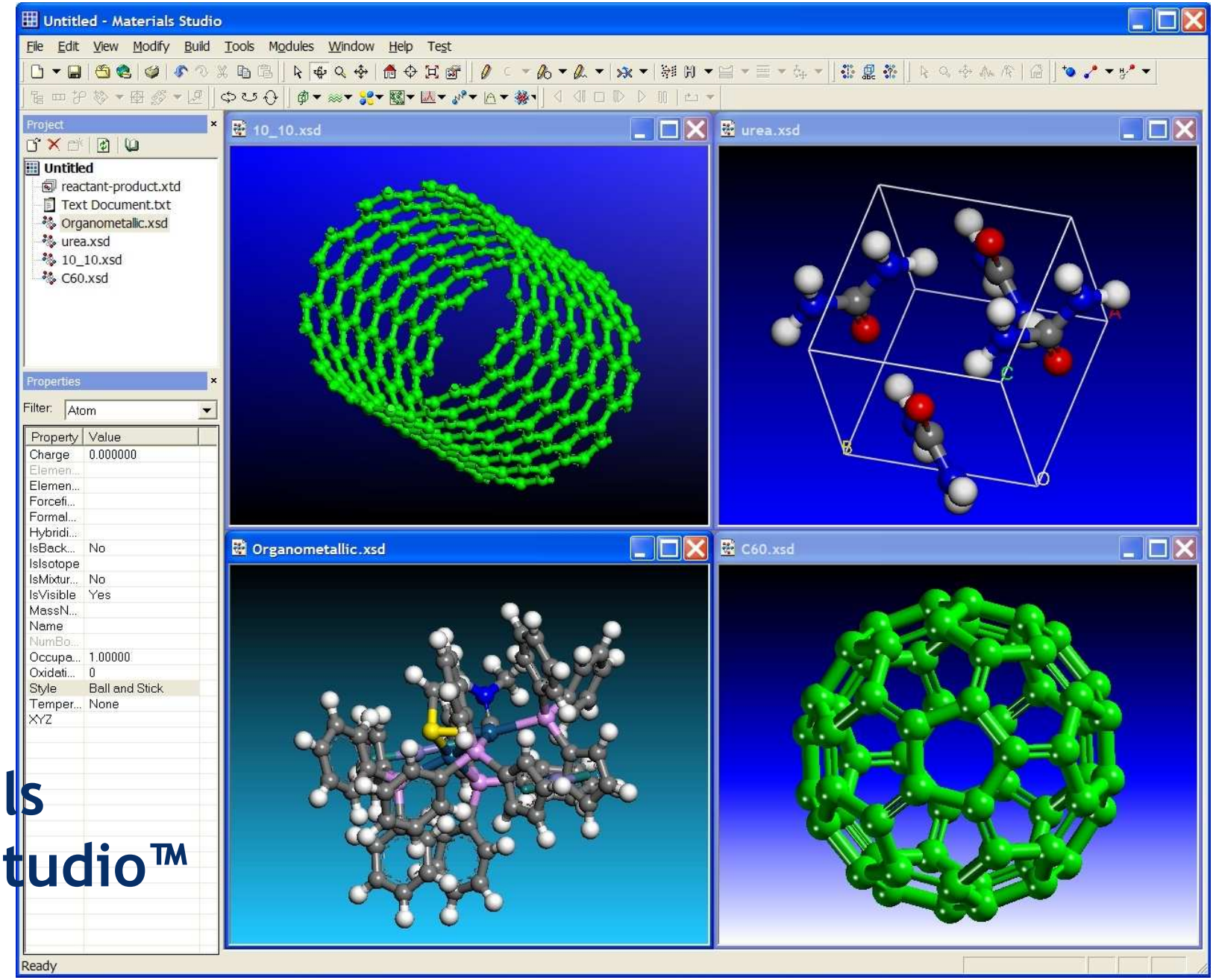
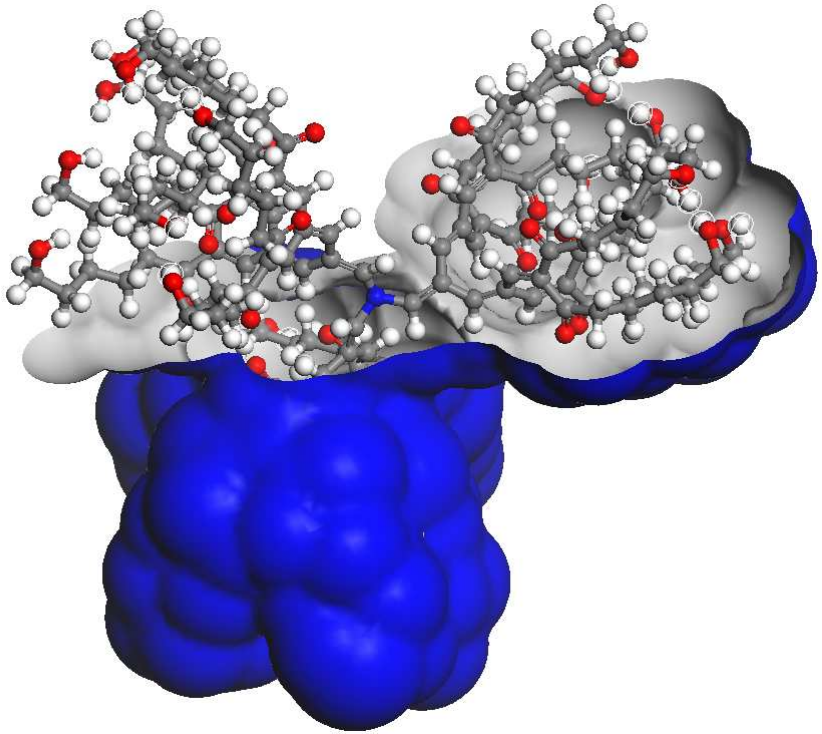
Modelling techniques unified in a software environment :



Materials Studio™

Materials Visualizer

- Atom Volumes
  - Molecules and 3D structures
- Atom numbering
- Study table (spreadsheet)



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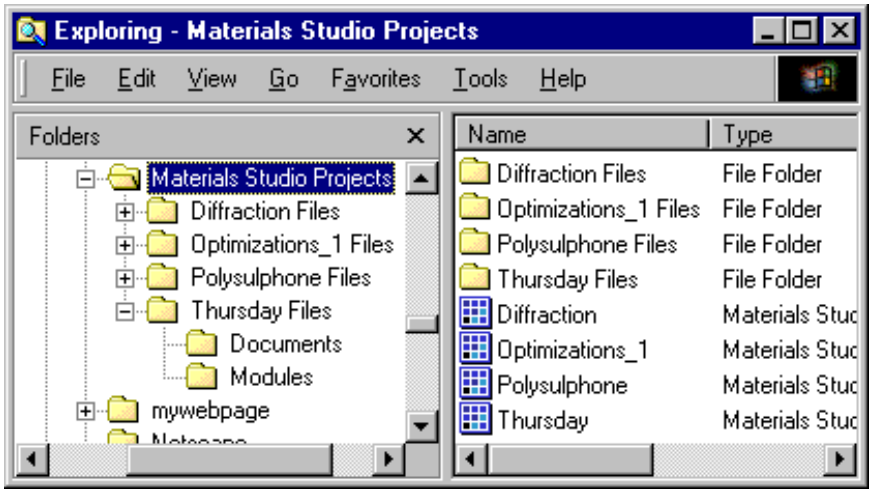
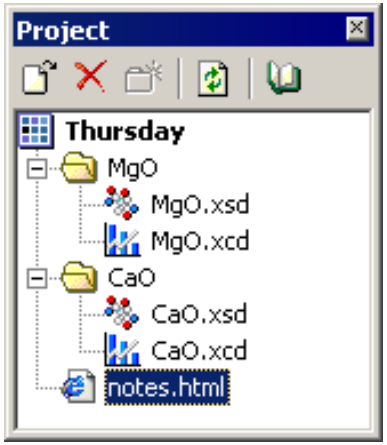
Materials Studio Projects

- All modeling is done within a project
  - **Data is managed for you**
- Projects contain
  - Documents
  - Applications state
- Projects are stored on disk in simple folder structure
  - hierarchical
  - easily maintained
- Projects can be shared
  - shared disks
  - zip and mail





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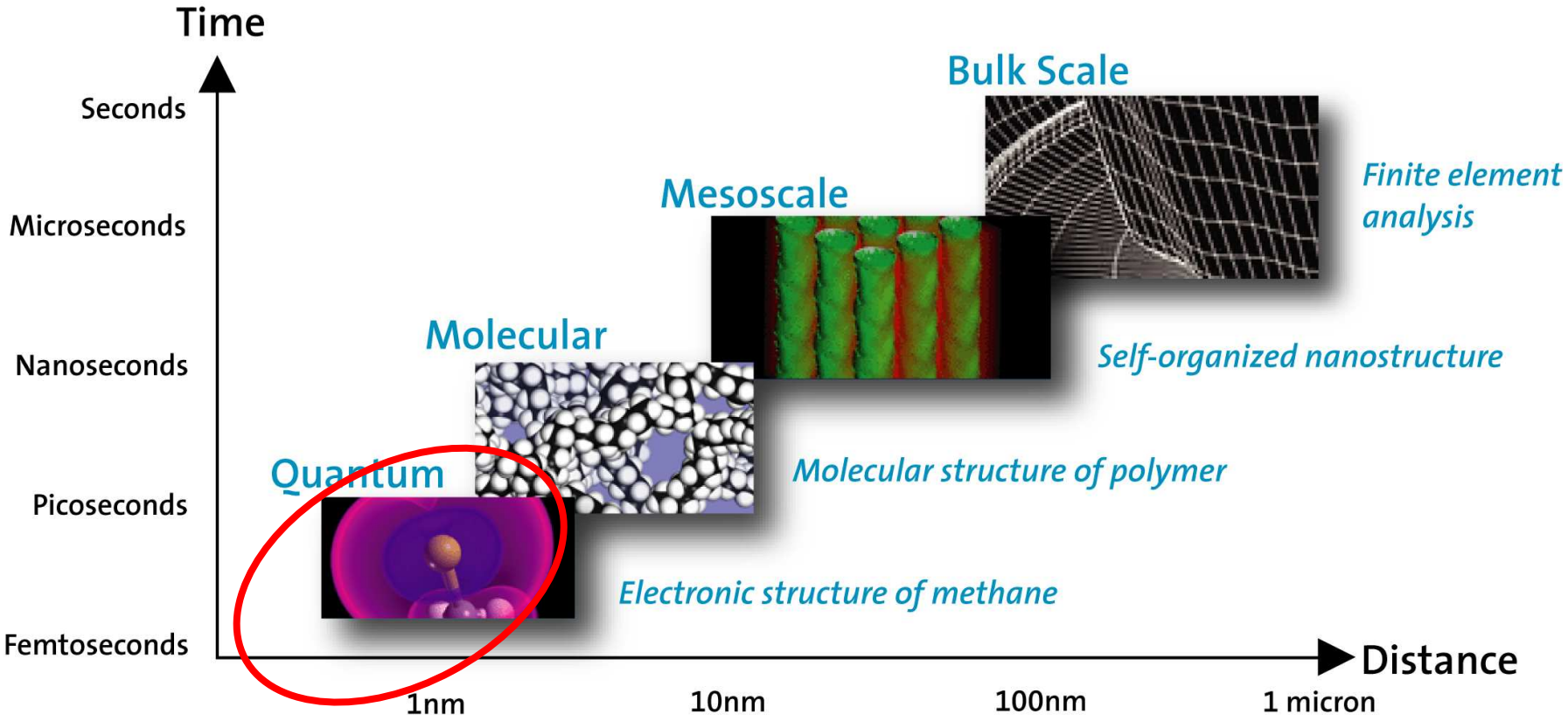
MS Modeling: A Complete Range of Methods



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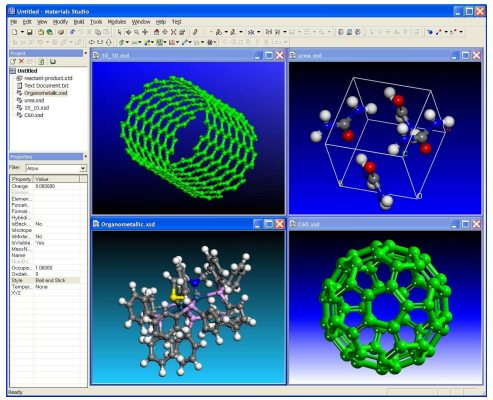
The Materials Modeling Environment



- Quantum Mechanics:
  - DMol^3 – ab initio QM simulation and analysis for Molecular and solid state
  - CASTEP – ab initio QM simulation and analysis for solid state
  - VAMP – semi-empirical quantum chemistry for molecules and nanoclusters

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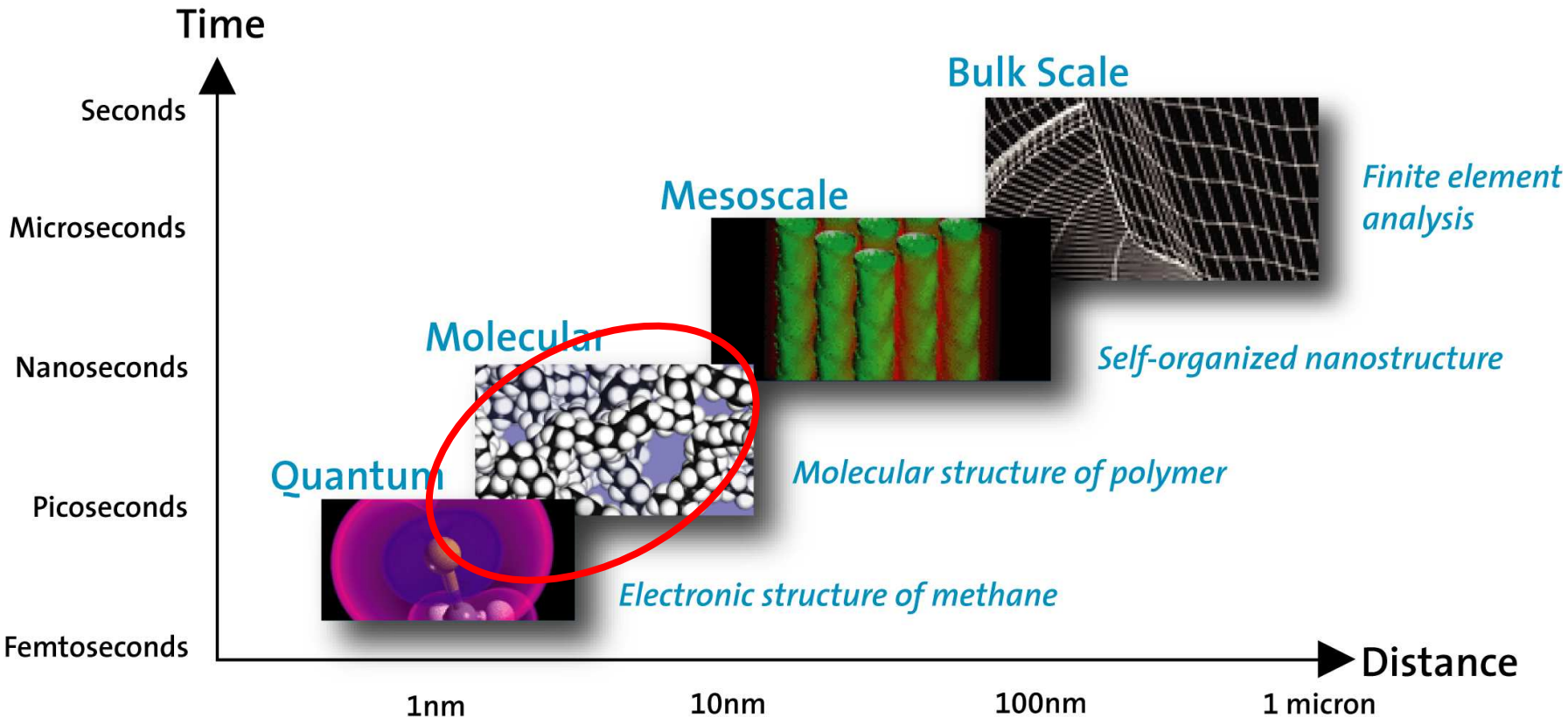
MS Modeling: A Complete Range of Methods



MATERIALS STUDIO

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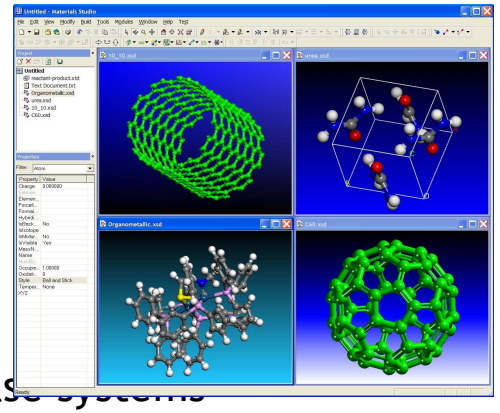
The Materials Modeling Environment

Materials Studio™



- Atomistic:
  - **Discover** - Simulation engine with analysis
  - **COMPASS** - Forcefield for simulation of condensed phase systems
  - Amorphous Cell - Modeling and analysis of bulk amorphous systems
  - Equilibria - Determination of phase diagrams and other thermodynamic data
  - **Forcite (Forcite+)** – Minimizaton and dynamics covering the full periodic table

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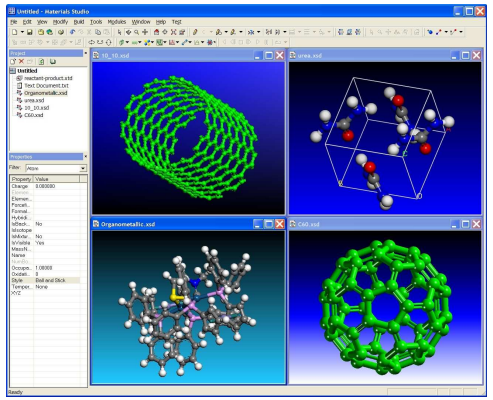
The Materials Modeling Environment



- Crystallisation and Growth:
  - Reflex - Powder diffraction simulation and analysis
  - Reflex Plus - For complete structure solution from powder diffraction data
  - Morphology – Crystal Morphology Prediction from structure data
  - Polymorph Predictor – Prediction of polymorphs from molecular structure data

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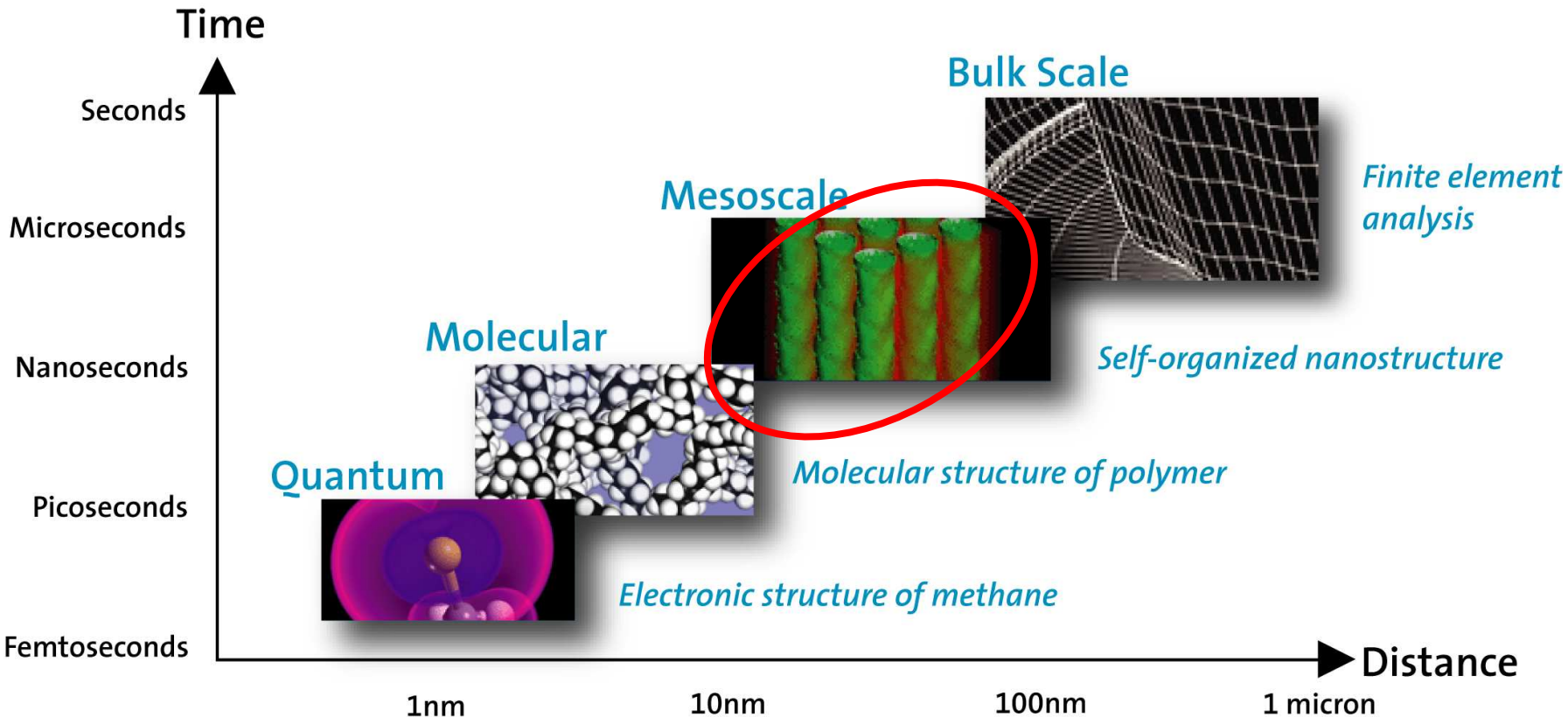
MS Modeling: A Complete Range of Methods



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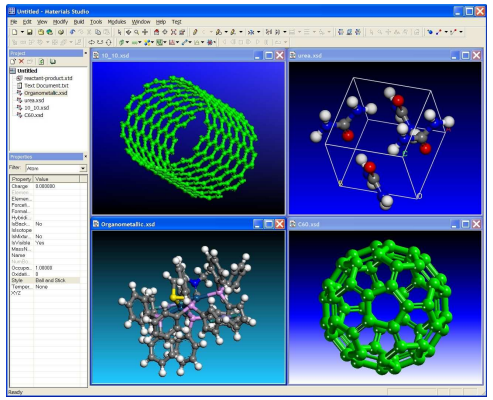
The Materials Modeling Environment
Materials Studio™



- Mesoscale:
  - MesoDyn - a dynamic simulation method for studying the long length and time behavior of complex fluid systems, including polymer melts and blends
  - DPD - (Dissipative Particle Dynamics) is a state of the art mesoscale simulation method for the study of complex fluids

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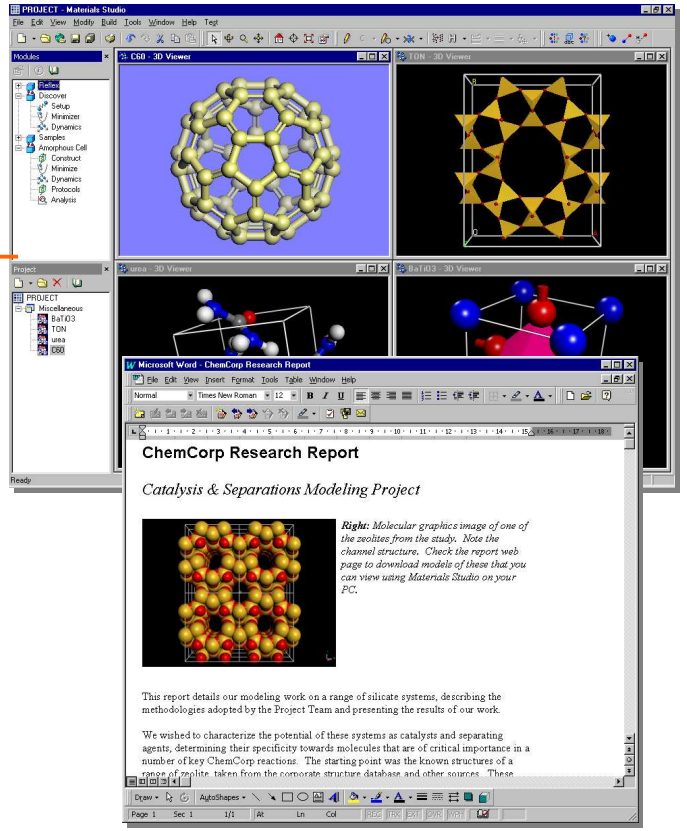
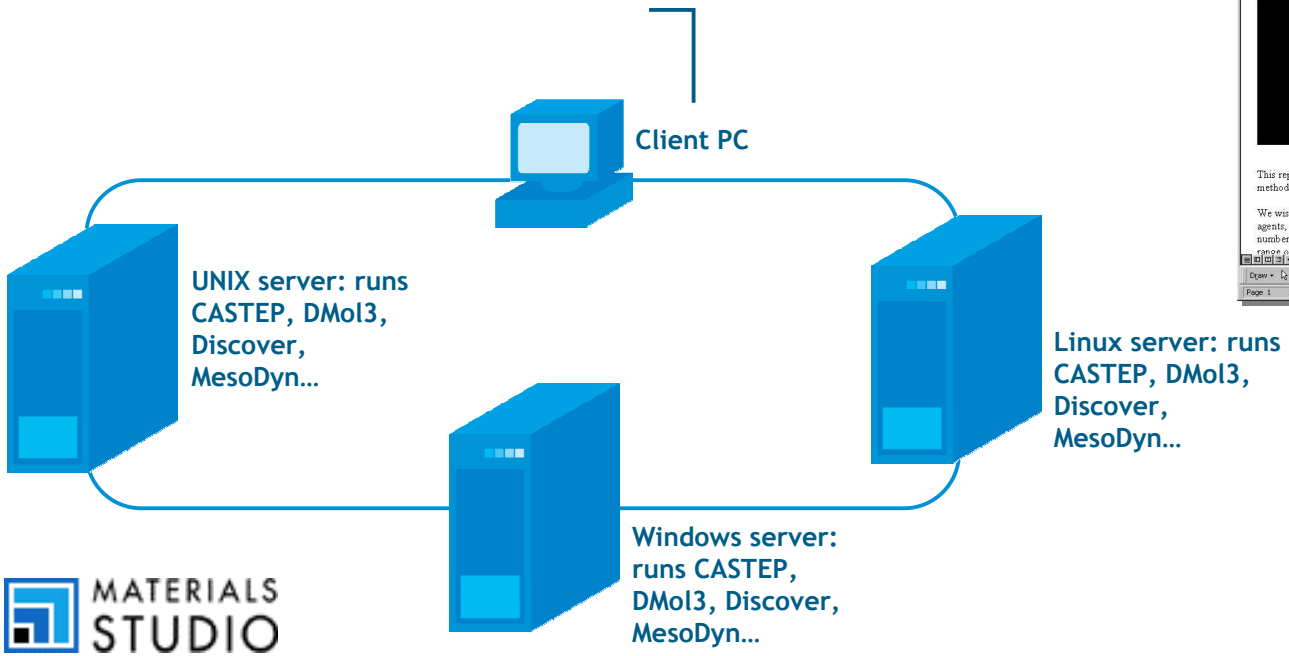
The Materials Studio Environment

A comprehensive range of applications with:

- Client-server computing





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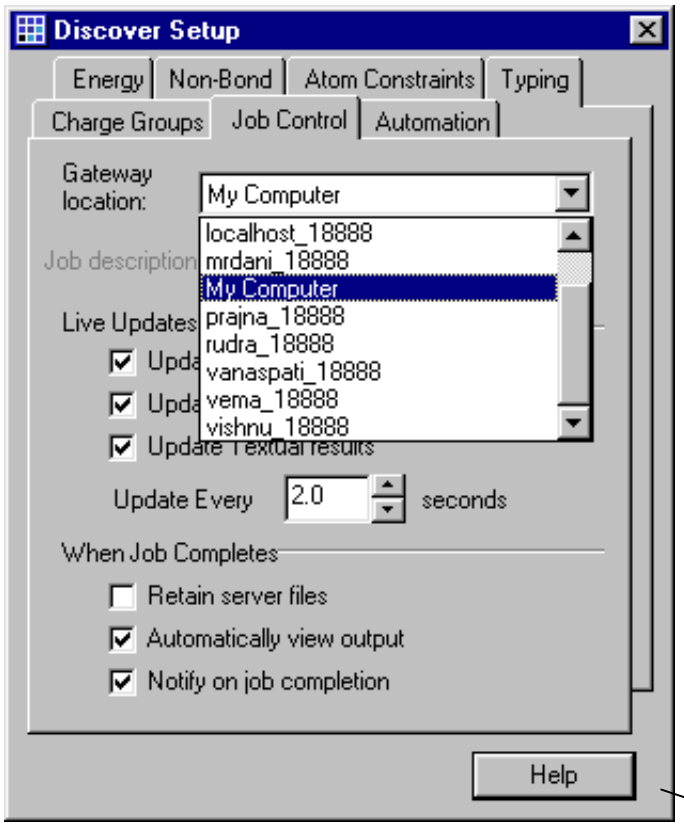
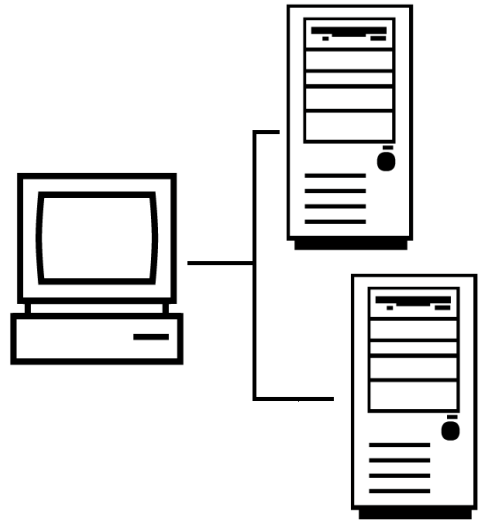
The Client-Server Architecture



Typical job control panel



Client PC

NT/2000, Linux, Irix, Tru64 servers

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Non-graphical server

- CPU intensive tasks
  - Discover, Amorphous Cell, Equilibria, DMol^3, CASTEP, Powder Solve

  - SGI Irix 6.5.4 and above
  - Windows NT4, SP4 and above, 2000, XP
  - Linux Redhat 6.0 and above
  - Compaq Tru64

  - SMP/MPI for certain codes

  - Intel partner ISV for Itanium

You can continue to use existing SGI hardware

- Multiple jobs on multiple servers

- Doesn't tie up client like Cerius^2

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