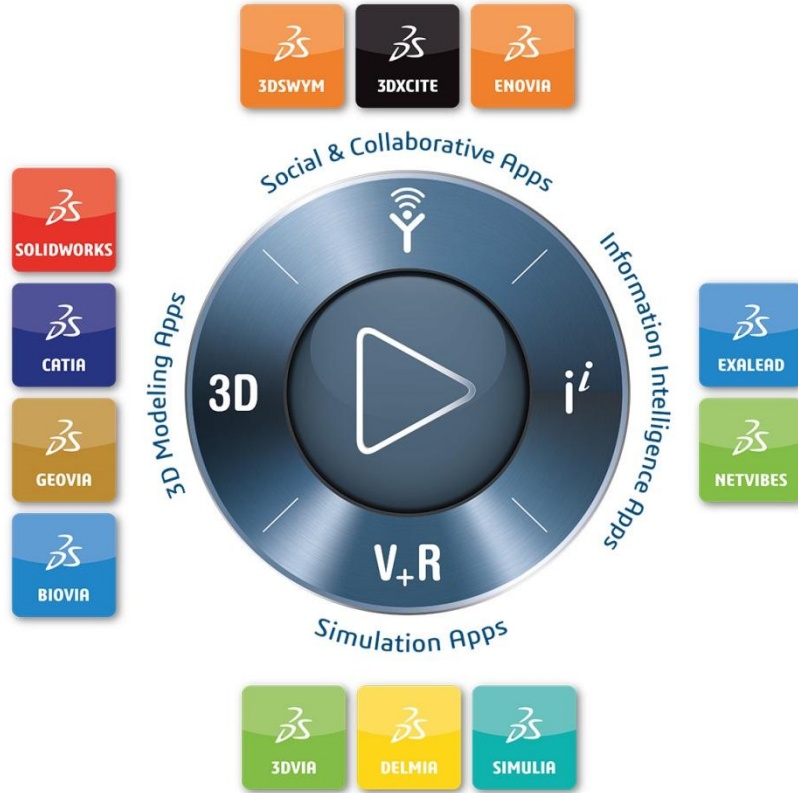




Material Studio Multi-scale Modelling Solutions

3DEXPERIENCE®

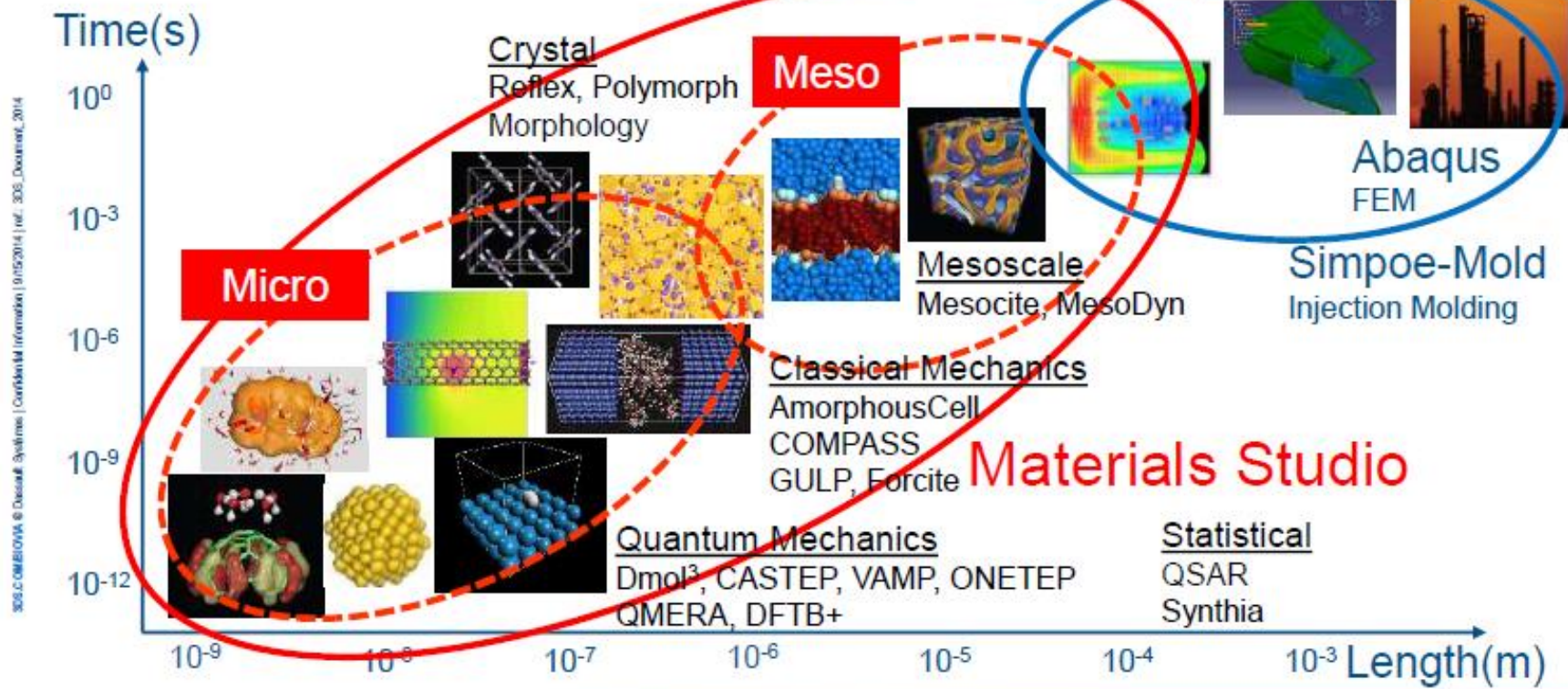


Our Clients

Industry Leaders at the Heart of Innovation

	CHEMICAL	     
	TRANSPORTATION & MOBILITY	        
	AEROSPACE & DEFENSE	    
	MARINE & OFFSHORE	    
	INDUSTRIAL EQUIPMENT	    
	HIGH-TECH	     
	CONSUMER GOODS - RETAIL	     
	CONSUMER PACKAGED GOODS - RETAIL	    
	LIFE SCIENCES	    
	ENERGY, PROCESS & UTILITIES	   
	ARCHITECTURE, ENGINEERING & CONSTRUCTION	    
	FINANCIAL & BUSINESS SERVICES	    
	NATURAL RESOURCES	    

Multiscale simulation of materials



3DS-COMBIOVIA © Dassault Systemes | Confidential Information | 01/15/2014 | ref.: 3DS_Document_2014

Theoretical Foundation

$$\mathbf{H} \Psi = E \Psi$$

Hamiltonian operates on wavefunction
of *all* electronic degrees of freedom

$$\left\{ -\frac{\hbar}{2m} \nabla^2 + V(\{\mathbf{r}_i\}) \right\} \Psi(\{\mathbf{r}_i\}) = E \Psi(\{\mathbf{r}_i\})$$

In practice, wave functions are expressed in
terms of one particle functions

$$\Psi(\{r_i\}) = F[\{\Phi_i\}]$$



Erwin Schrödinger

Density Functional Theory

- Exact only for ground state
- Needs approximation to E_{xc}



Walter Kohn

Hohenberg-Kohn theorem

$$E[\Psi(\vec{r}_1, \dots, \vec{r}_N)] = E[\rho(\vec{r})]$$

$$E[\rho] = T_o[\rho] + U[\rho] + E_{xc}[\rho]$$

Kohn-Sham theorem

$$\left. \frac{\partial E[\rho]}{\partial \rho} \right|_{\rho=0} = 0$$

Kohn-Sham equations

$$\left[\nabla^2 + v_{eff}[\rho(\vec{r})] \right] \varphi_{i,\vec{k}}(\vec{r}) = \varepsilon_{i,\vec{k}} \varphi_{i,\vec{k}}(\vec{r})$$

DMol³: Linear Combination of Atomic Orbitals

$$\psi_i = \sum_{\alpha} \sum_j c_{ij}^{\alpha} \phi_j^{\alpha}(r_{\alpha})$$

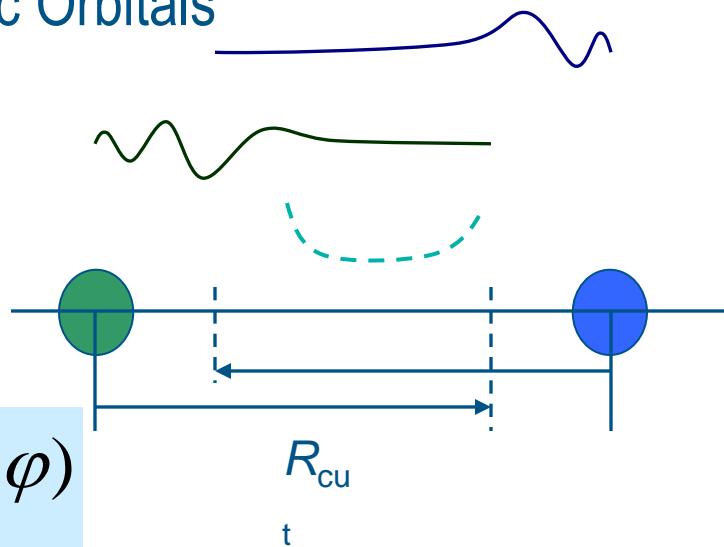
$$\phi_j^{\alpha}(r_{\alpha}) = \sum_{lm} \underbrace{R_{nl}^{\alpha}(r)}_{\text{Radial portion}} \underbrace{Y_{lm}(\vartheta, \varphi)}_{\text{Angular Portion}}$$

Radial portion
atomic DFT eqs. numerically

Angular
Portion

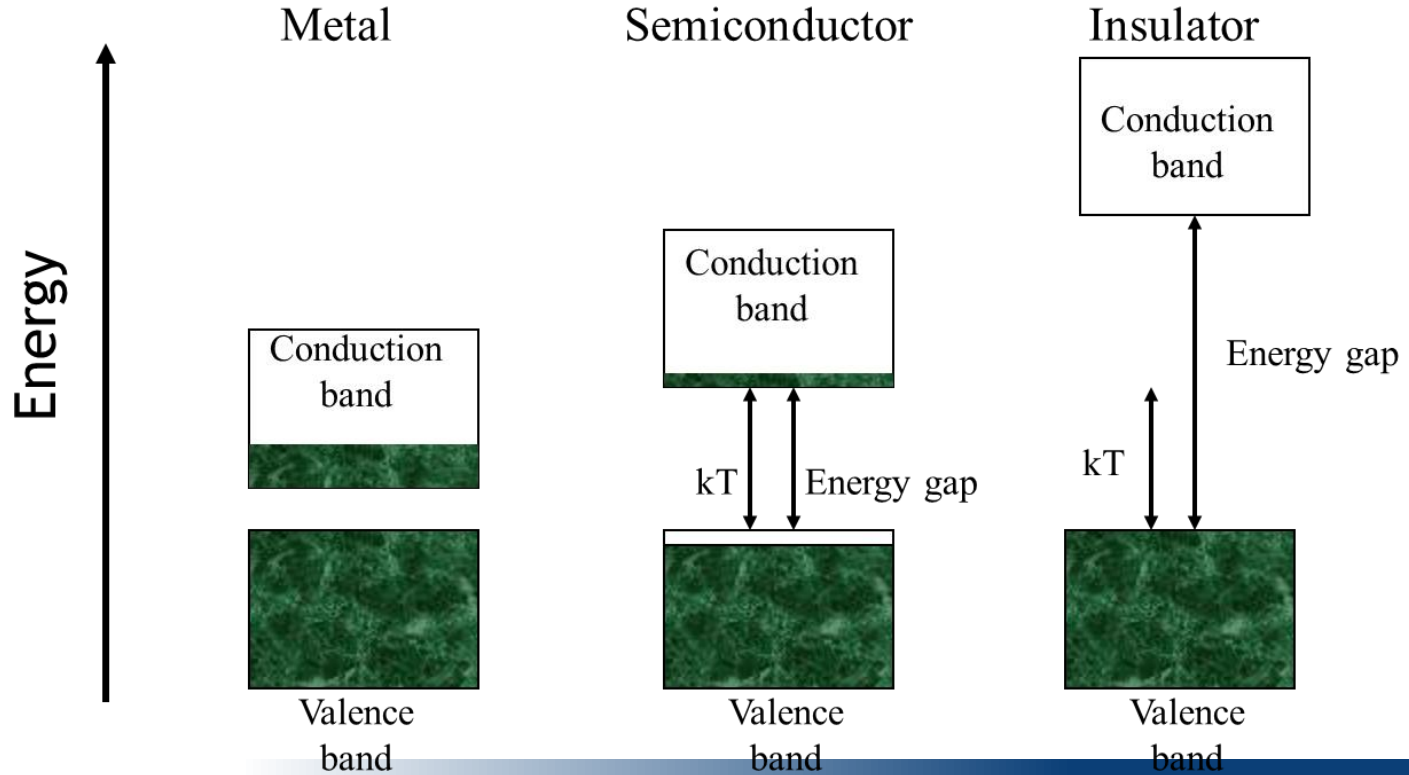
Periodic and
aperiodic
systems

Good for molecules, clusters, zeolites, molecular crystals, polymers "open structures"



Mind the gap!

Solids can be divided in three classes based upon their band structure



What are the mathematical solvers for materials ?

Schrodinger equation Solvers Based on Quantum Mechanics

Wave function based Methods

Gaussian Basis (Gaussian, MOLCAS)

Numerical Basis (**DMOL3**, FHI-AIMS) or

Mixed Plane Wave and
Gaussian Basis (CP2K)

Popular with Chemists

Semi – Empirical

Overlap approximation methods
VAMP

Popular with Chemists

Hybrid Classical-Quantum

QMERA

Plane Wave Based Methods

Pseudopotential Approach
(CASTEP)

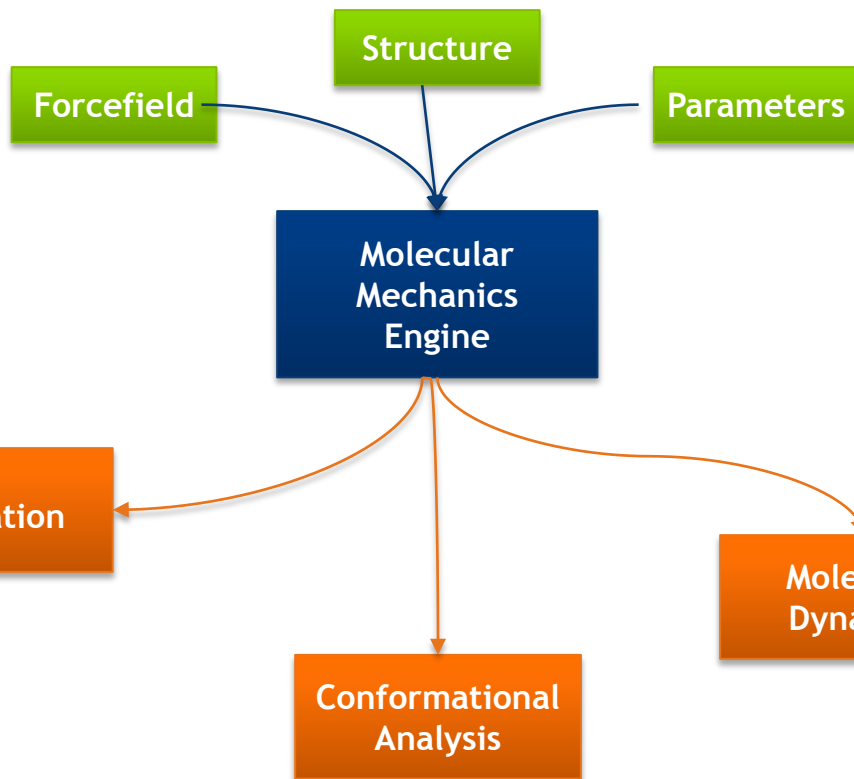
Tight Binding (DFTB+)

Wannier Functions (ONETEP)

Popular with Physicists
(Condensed Matter Physics)

Density Functional Theory with
Material Studio

Molecular Mechanics



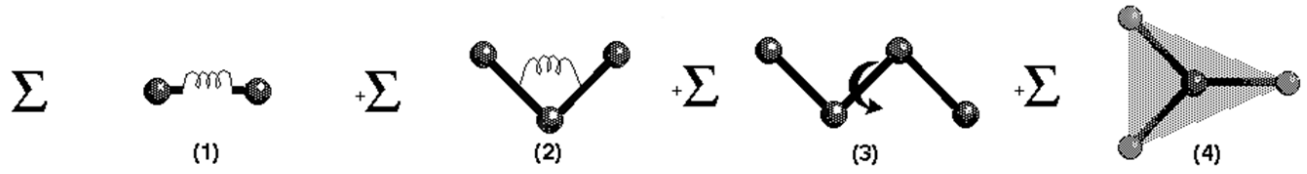
Pros

- Based on Newtonian mechanics
- Intuitive to Engineers
- Simplistic treatment using springs

Cons

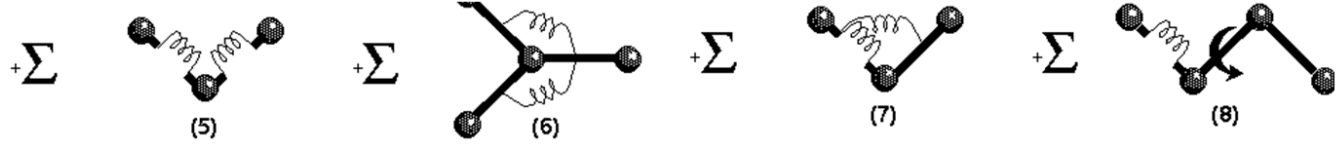
- Hardcoded and extensively parameterized sets required (usually non transferable)
- Bond dissociation is not defined (except ReaxFF), hence no reactions

Representation of a forcefield - Part 2

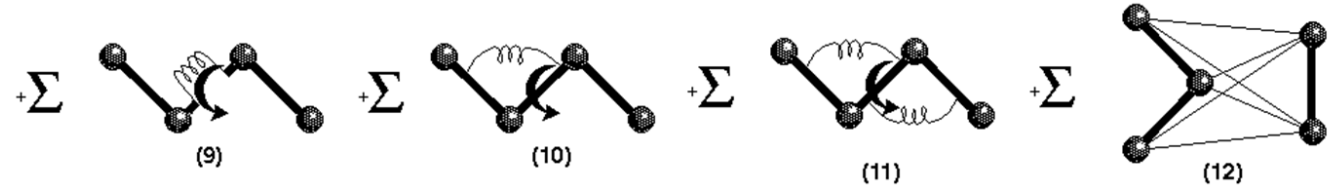


$$\sum_b [K_2(b-b_0)^2 + K_3(b-b_0)^3 + K_4(b-b_0)^4] + \sum_{\theta} K_z z^2$$

$$+ \sum_{\theta} H_2(\theta-\theta_0)^2 + H_3(\theta-\theta_0)^3 + H_4(\theta-\theta_0)^4 + \sum_{\phi} [V_1[1-\cos(\phi-\phi_0^0)] + V_2[1-\cos(2\phi-\phi_0^0)] + V_3[1-\cos(3\phi-\phi_0^0)]]$$



$$+ \sum_b \sum_{b'} F_{bb'}(b-b_0)(b'-b'_0) + \sum_{\theta} \sum_{\theta'} F_{\theta\theta'}(\theta-\theta_0)(\theta'-\theta'_0) + \sum_b \sum_{\theta} F_{b\theta}(b-b_0)(\theta-\theta_0) + \sum_b \sum_{\phi} (b-b_0)[V_1 \cos \phi + V_2 \cos 2\phi + V_3 \cos 3\phi]$$



$$+ \sum_{b'} \sum_{\phi} (b'-b'_0)[V_1 \cos \phi + V_2 \cos 2\phi + V_3 \cos 3\phi] + \sum_{\theta} \sum_{\phi} (\theta-\theta_0)[V_1 \cos \phi + V_2 \cos 2\phi + V_3 \cos 3\phi] + \sum_{\phi} \sum_{\theta} \sum_{\theta'} K_{\phi\theta\theta'} \cos \phi (\theta-\theta_0)(\theta'-\theta'_0) + \sum_{i>j} \frac{q_i q_j}{\epsilon r_{ij}} + \sum_{i>j} \left[\frac{A_{ij}}{r_{ij}^9} - \frac{B_{ij}}{r_{ij}^6} \right]$$

What are the mathematical solvers for materials ?

Classical Mechanics Solvers are based on Force Fields

Methods for Soft Condensed Matter
(Polymers, foams, amorphous materials)

Forcite

UNIVERSAL: Rule Based
Dreiding, CVFF: Gen 1 FF
PCFF, **COMPASS: Gen 2 FF**

Methods for Inorganic Solids
(Crystalline state)

GULP

Shell Models

Coarse Grained
Mesoscale Methods

Mesocite

Industry benchmarked standards

System Models

- Polymers
 - Engineering Polymers
 - Fuel cell Polymers
 - Nanocomposites
 - Surfactant
 - Drug delivery polymers
- Blends & Formulations
- Microporous materials

- Minerals, Oxides
- Metals, Alloys
- Heterogenous & Homogenous Catalysts
- Solvents
- Ceramics & Inorganic Glass
- Semiconductors
- Agrochemicals & Drugs

Process Simulations

- Adsorption/Absorption
- Separation/Diffusion
- Reaction/Interaction
- Adhesion/Cohesion
- Annealing
- Surfaces/Interfaces
- Mechanical/Thermal process

- Miscibility/Solubility
- Stabilization
- Dispersion
- Corrosion inhibition
- Equilibrium
- Polymorphism

Statistical correlations

- Identify the factors critical to Process and predict optimal behavior
- Better quality systems, reduced experiment
- Optimize formulated products and reduce experimental costs

System data management & analysis

- Sample quality/purity
- Literature data on system of interest
- Process conditions

In Silico Property Prediction

- Remove unnecessary synthesis – save money
- Assess properties – reduce experiment and risk

Testing

- Focus experiment on the most productive pathways

CHARACTERIZATION

IMPROVE PROCESS

OPTIMIZED PROCESS

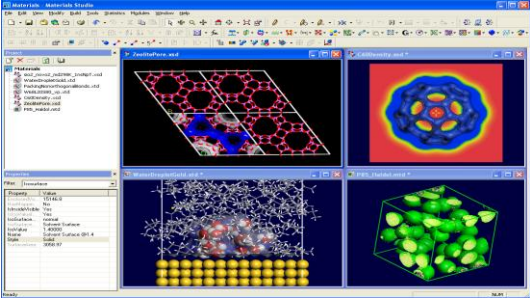
Analytical Simulations

- Spectroscopic
 - UV-Visible
 - Vibrational
 - NMR
- Structural
 - XRD, Morphology, Crystallization

Product

Materials Studio extension to connect with the experimental world

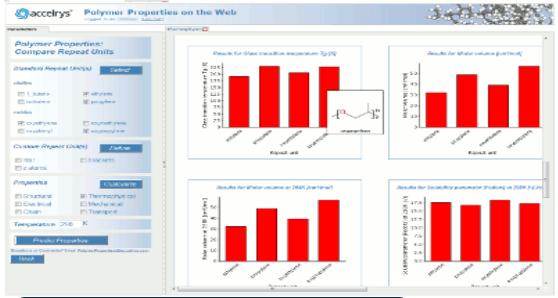
Windows
CLIENT



Materials Visualizer



PP Pro Client
(assembly/automation)



Pipeline Pilot Web
(deployment)

Windows
or Linux
SERVER

Materials Studio Gateway

Pipeline Pilot Server



How does it WORK !

3 D VISUALIZER

Sketch & Build, Polymers Crystals Layers, Monte-Carlo, 3D Surface, Electrodes

Quantum Mechanics

Classical Mechanics

Meso Scale

INFORMATICS

DMOL³

CASTEP

FORCITE

GULP

MESOCITE

QSAR

SYNTHIA

ONETEP

DFTB+

CONFORMERS

XRAY

DPD

MODELS
Genetic & Neural

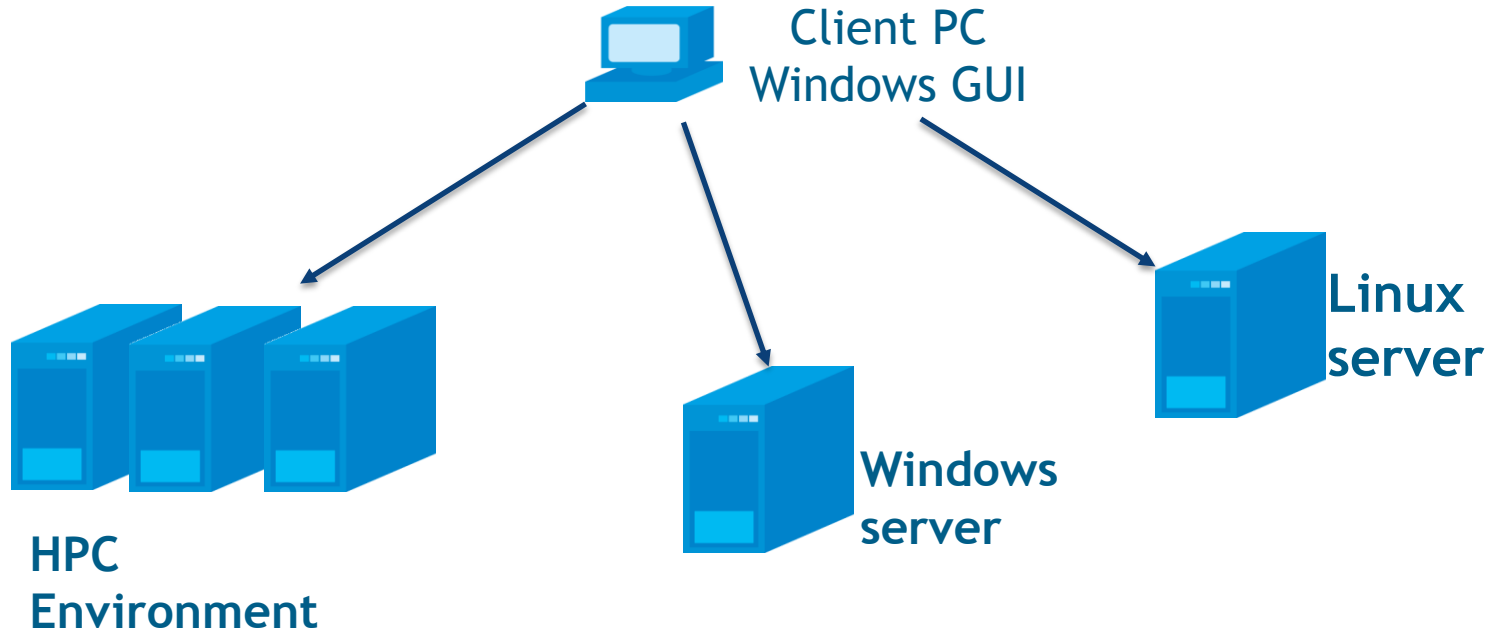
VAMP

QMERA

Proprietary COMPASS Force Field
NOW Gen. 2

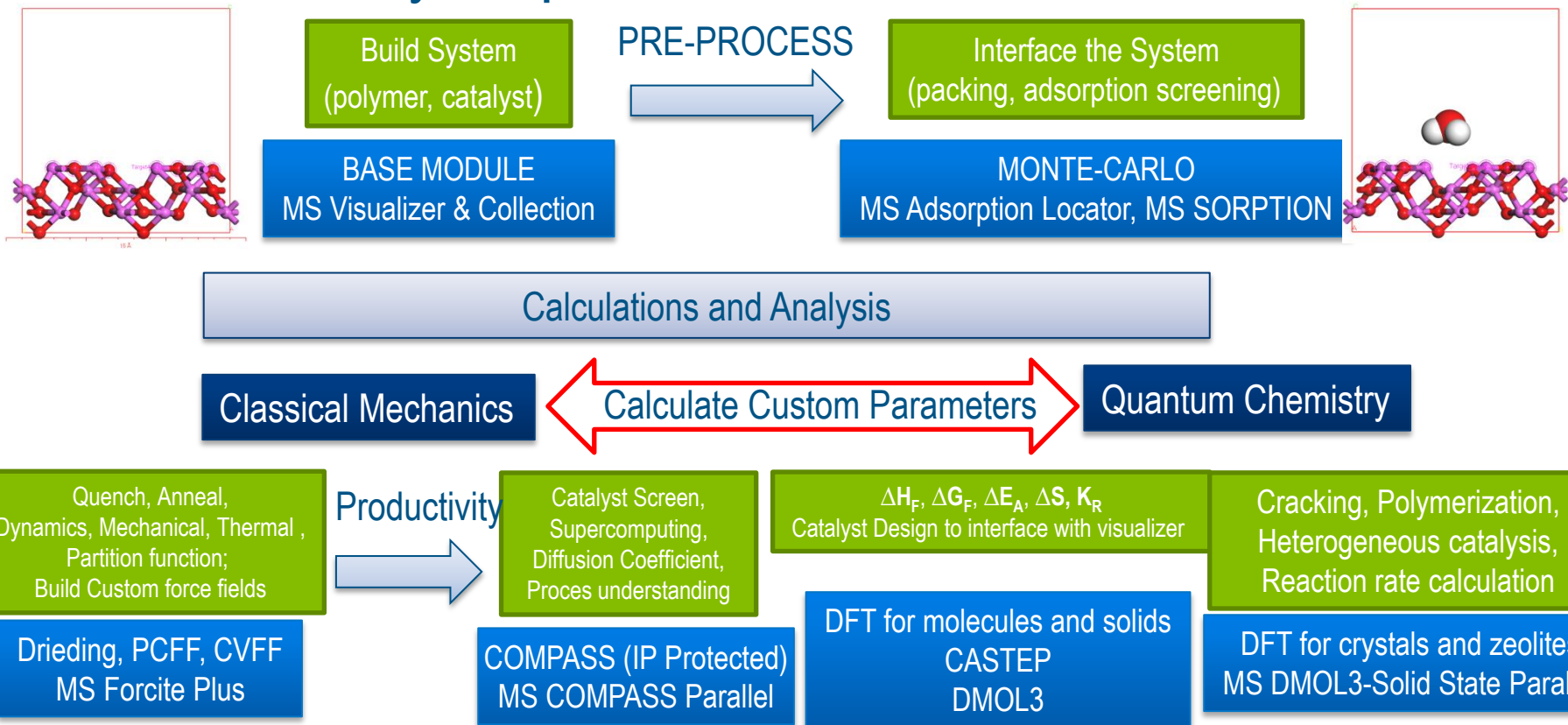
Perl Scripting, Parallelization framework, Connectivity

Client-server architecture



NOTE: The client machine can also be configured to be a server machine

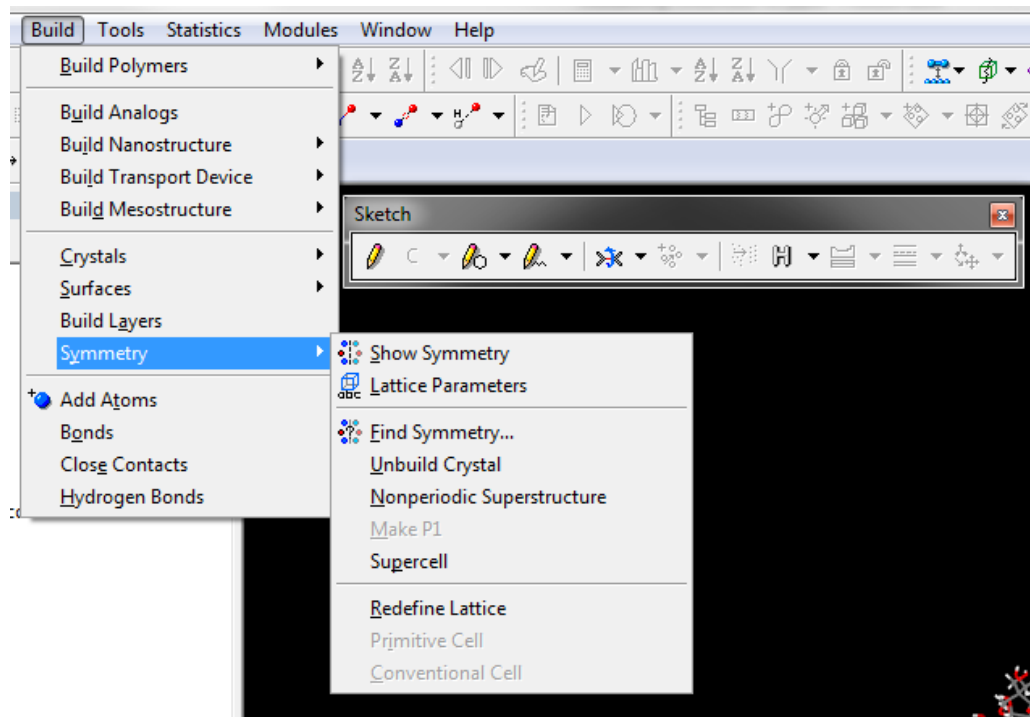
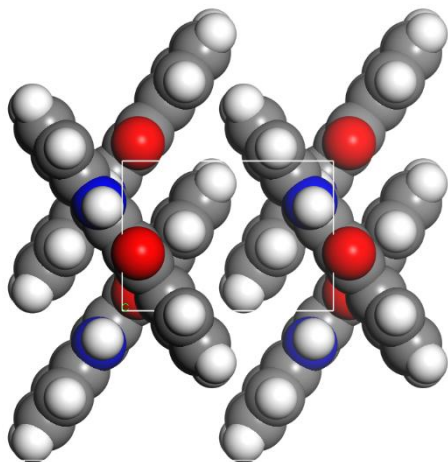
Functionality Map for Materials Studio Modules



System Build and Sketch

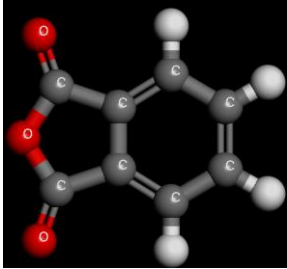
Sketch & BUILD

BASE MODULE
MS Visualizer & Collection

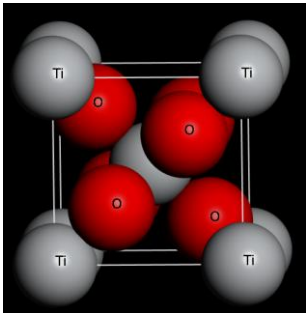


System Build and Sketch

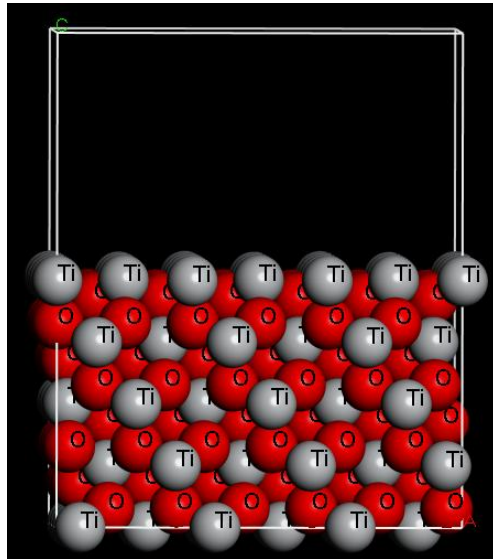
Simple Molecules
Clusters Complexes



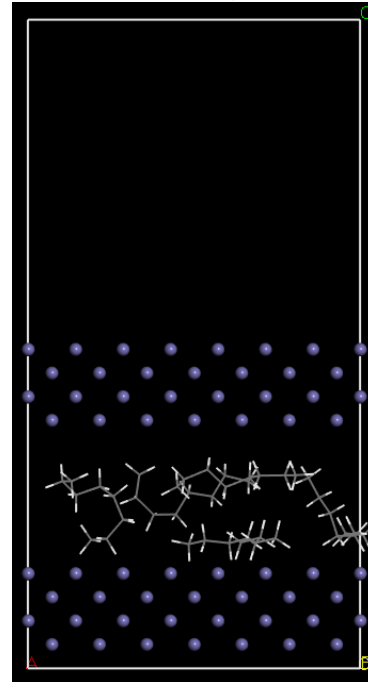
Crystals
Inorganic/Molecular



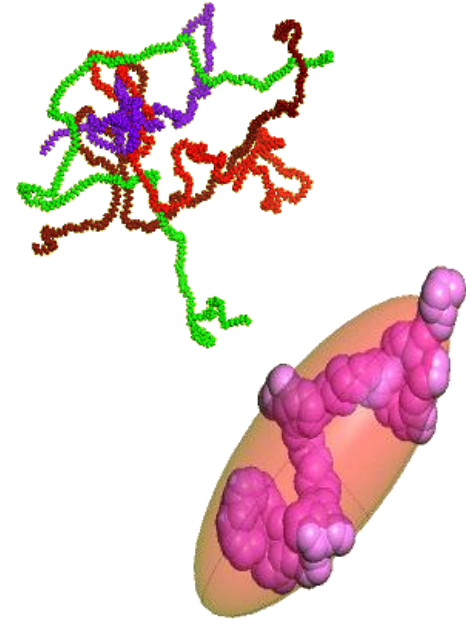
Cleave Crystals
Build Interfaces



Build Layers
Build Polymers

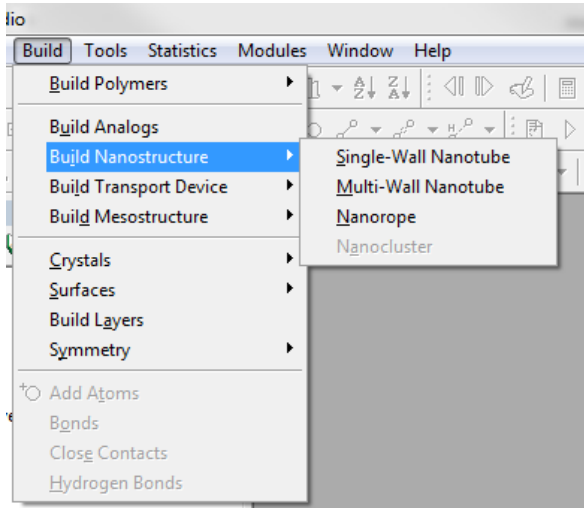


Build Meso-
Structures

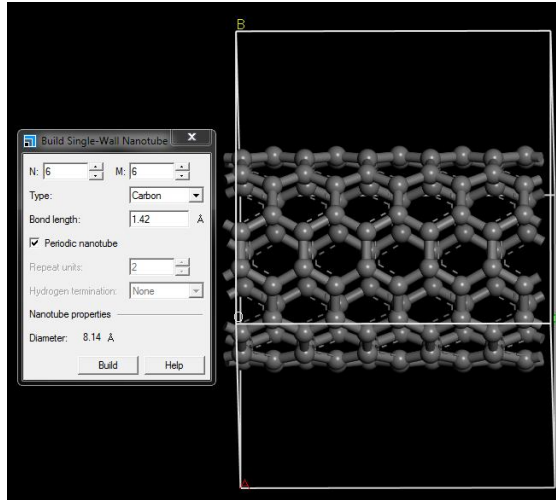


System Build and Sketch: Build Nanostructures

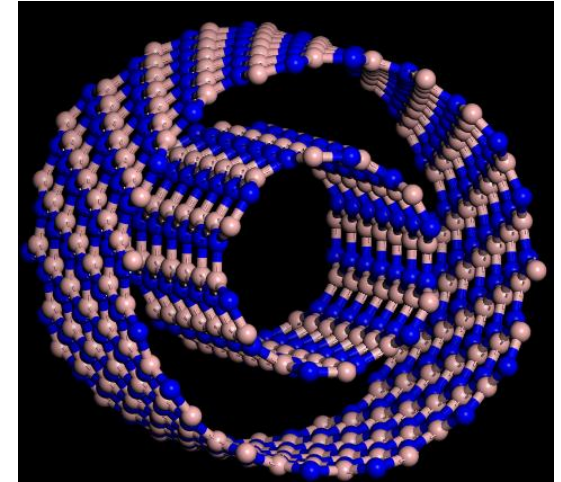
Nano Builder Options



Single Walled Carbon Nanotube



Multi Walled Boron Nitride Nanotube



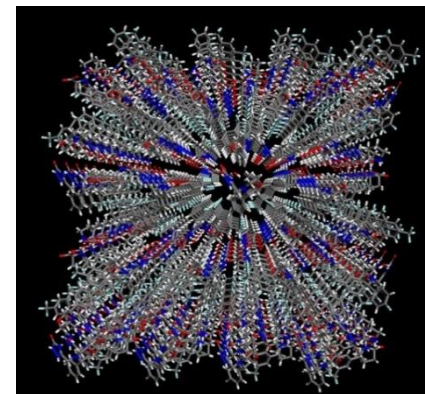
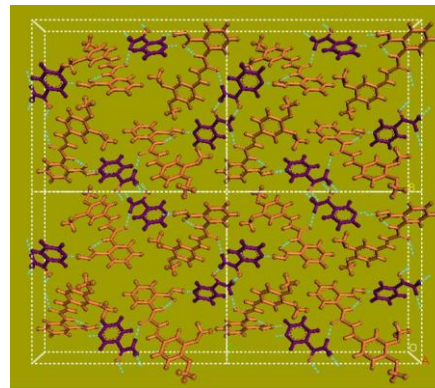
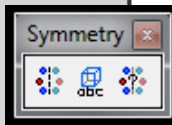
Crystal Building

Crystal Building

- Build Crystals & Surfaces
- Import Files – e.g. from CCDC Conquest

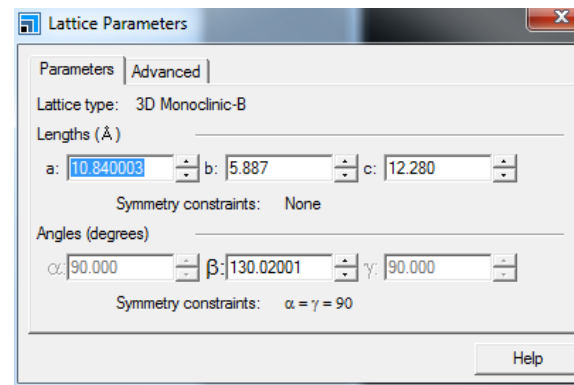
Symmetry

- Show and find symmetry
- Lattice parameters



Visualize

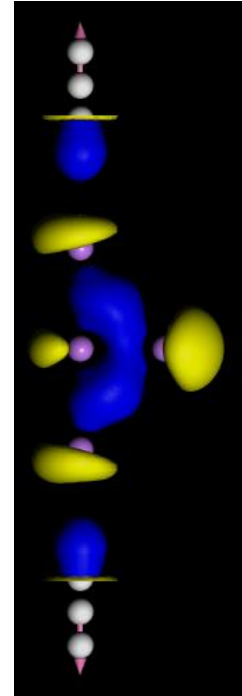
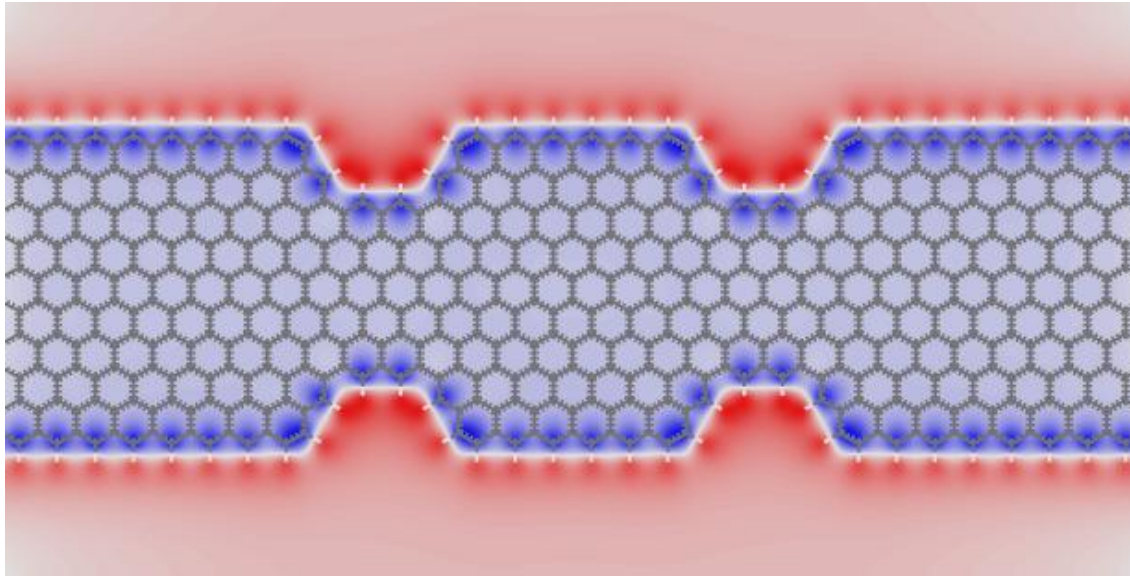
- Display style
- Hydrogen bond
- Distance & Angles monitors
- Cleave surface
- Display miller planes



System Build and Sketch: Build Transport Device

Build Electrode

Build Transport Device like polymer, molecule



Pre-Processing and screening

Interface the System
(packing, adsorption screening)

MONTE-CARLO
MS Amorphous Cell
MS Adsorption Locator
MS SORPTION

MS Amorphous Cell

Build your system (polymer/molecule/solvent) by packing it into various boxes or within molecules/ cavities/ surfaces.

MS Adsorption Locator

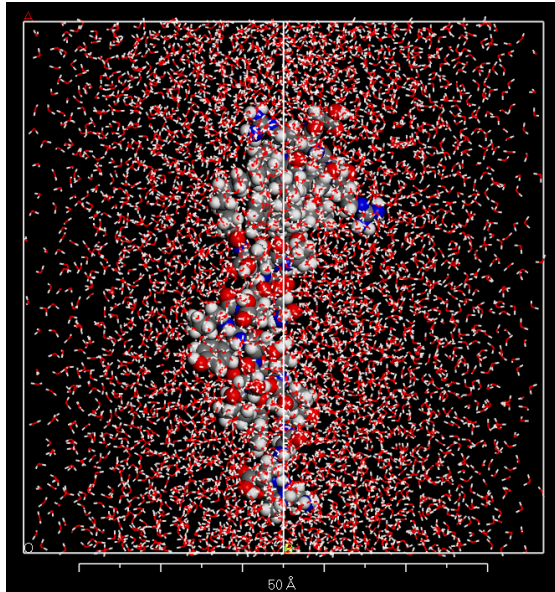
A built system has to interface with a reactant or catalyst. Heterogeneous catalyst adsorption is performed via Monte-Carlo steps on the adsorbate to quickly screen through the configuration space. Works for both periodic and non-periodic structures and delivers low energy geometry.

MS SORPTION

An adsorbate can interact with a 3D porous network like zeolite and nanostructures. For microporous framework one can calculate adsorption isotherms and Henry constants with this module. Especially to know where the adsorbed molecules are located within the nano-porous catalyst.

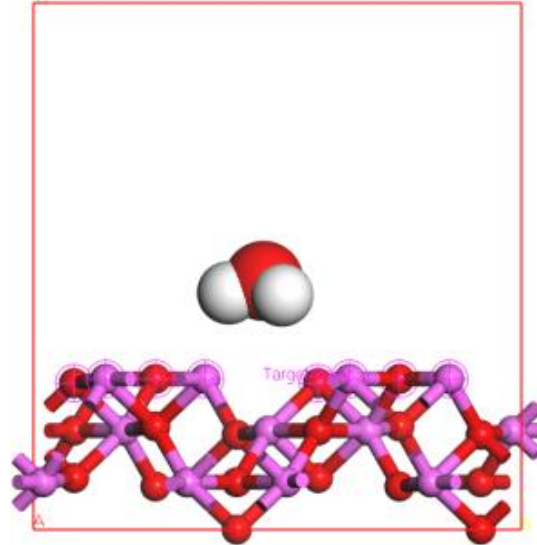
Pre-Processing and screening

Amorphous Cell Construction
and Solvent Packing

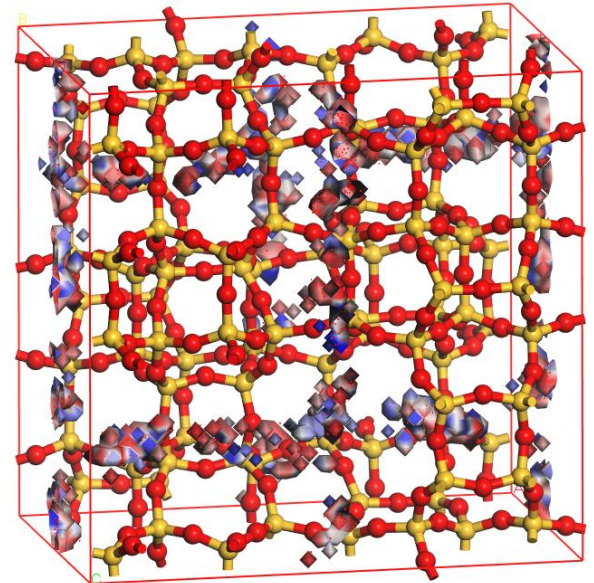


Find minimum energy
adsorption sites on the
crystal surface

MS Adsorption Locator



Calculate Adsorption sites
in Porous media
MS Sorption



MS Sorption

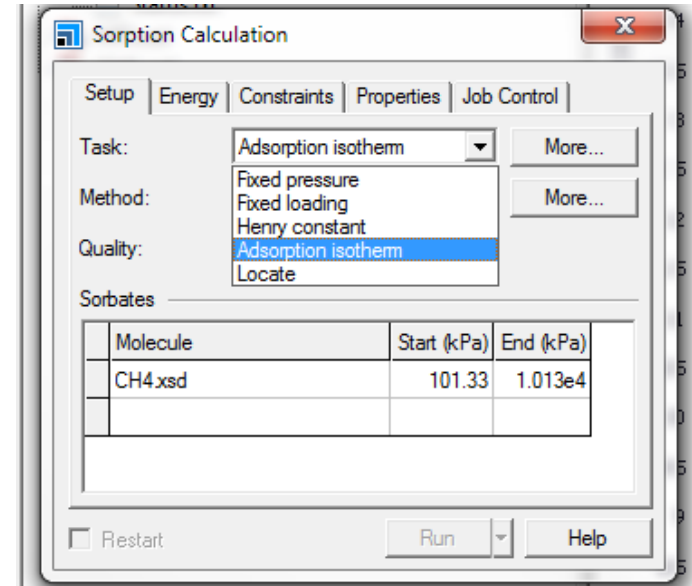
Henry Constant

$$H_i = \lim_{x_i \rightarrow 0} \frac{f_i}{x_i}$$

- Ratio of fugacity and the mole fraction of the solute at infinite dilution and zero pressure
- Quantify the affinity of a sorbate

Adsorption Isotherm

- Simulate a framework in open contact with a sorbate reservoir over a range of pressures at a given temperature
- The loading at each point in the pressure range is calculated and the points combined to create an isotherm



Calculations – Classical Mechanics

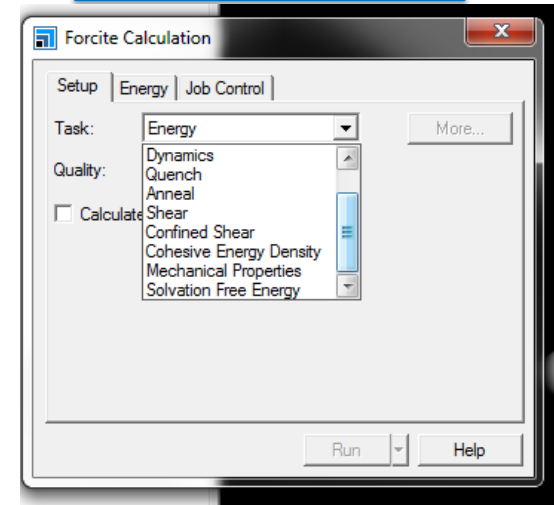
MS Forcite (Plus)

- Workhorse classical mechanics module
- Perform Force field based tasks such as Molecular Dynamics (all ensembles)
- Includes BIOVIA Proprietary COMPASS(II) force field along with Drieding, PCFF, CVFF, Universal and supports wide variety of atom types
- Ewald Summation and PPPM algorithm for electrostatic calculations

Classical Mechanics

Quench, Anneal,
Dynamics, Mechanical, Thermal ,
Partition function;
Build Custom force fields

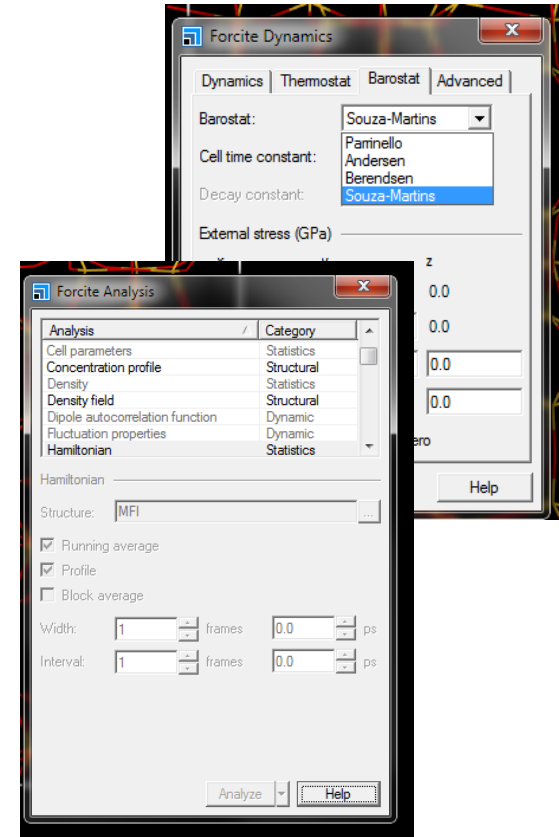
Drieding, PCFF, CVFF
MS Forcite Plus



Calculations – Classical Mechanics

MS Forcite (Plus) Analysis

- Analyse a wide variety of structural parameter evolution of the trajectory (auto-correlation, RDF, MSD, radius of gyration, etc)
- NVE, NVT, NPH NPT supported ensembles
- Parinello, Andersen, Berendsen and Souza-Martins supported Barostats
- Velocity rescaling, Nose, Andersen, Berendsen and NHL supported Thermostats
- Supports parallel calculations on HPC system



Calculations – Classical Mechanics

MS Forcite (Plus) – Force Field Manager

- Construct custom force fields
- Support for a wide variety of expressions
- Custom atom types
- Use charges calculated via quantum methods from the interface directly

Filter by selection in:

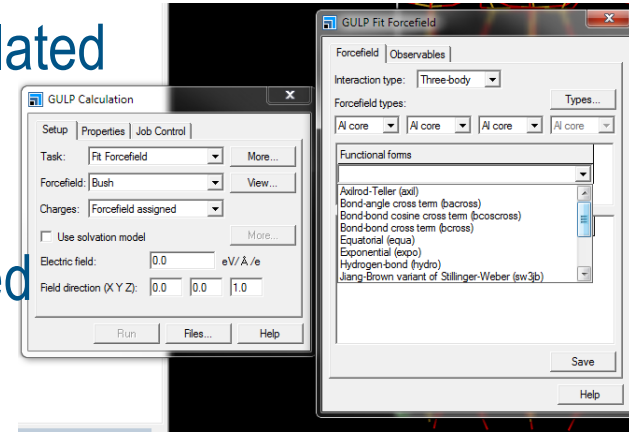
Type	Description	Element Symbol	van der Waals Form
Filter			All
Al3	aluminium	Al	LJ_12_6
As3	arsenic	As	Buckingham Ignore
B_2	boron, sp2	B	LJ_12_4
B_3	boron, sp3	B	LJ_12_6
Br	bromine	Br	LJ_12_6_X LJ_9_4 LJ_9_6 LJ_9_6_X
C_1	carbon, sp1	C	LJ_12_6
C_11	carbon, sp1, 1 implicit hydrogen	C	LJ_12_6
C_2	carbon, sp2	C	LJ_12_6
C_21	carbon, sp2, 1 implicit hydrogen	C	LJ_12_6
C_22	carbon, sp2, 2 implicit hydrogens	C	LJ_12_6
C_3	carbon, sp3	C	LJ_12_6
C_31	carbon, sp3, 1 implicit hydrogen	C	LJ_12_6
C_32	carbon, sp3, 2 implicit hydrogens	C	LJ_12_6
C_33	carbon, sp3, 3 implicit hydrogens	C	LJ_12_6
C_34	carbon, sp3, 4 implicit hydrogens	C	LJ_12_6
C_R	carbon, aromatic	C	LJ_12_6
C_R1	carbon, aromatic, 1 implicit hydrog	C	LJ_12_6
C_R2	carbon, aromatic, 2 implicit hydrog	C	LJ_12_6
Ca	calcium	Ca	LJ_12_6
Cl	chlorine	Cl	LJ_12_6
F_	fluorine	F	LJ_12_6
Fe	iron	Fe	LJ_12_6
Ga3	gallium	Ga	LJ_12_6
Ge3	germanium	Ge	LJ_12_6
H_	hydrogen	H	LJ_12_6
H__A	hydrogen, involved in hydrogen bc	H	LJ_12_6
H__b	hydrogen, bridging hydrogen	H	LJ_12_6
I_	iodine	I	LJ_12_6
In3	indium	In	LJ_12_6

Summary | Types | Interactions | Equivalences

Calculations – Classical Mechanics

MS GULP

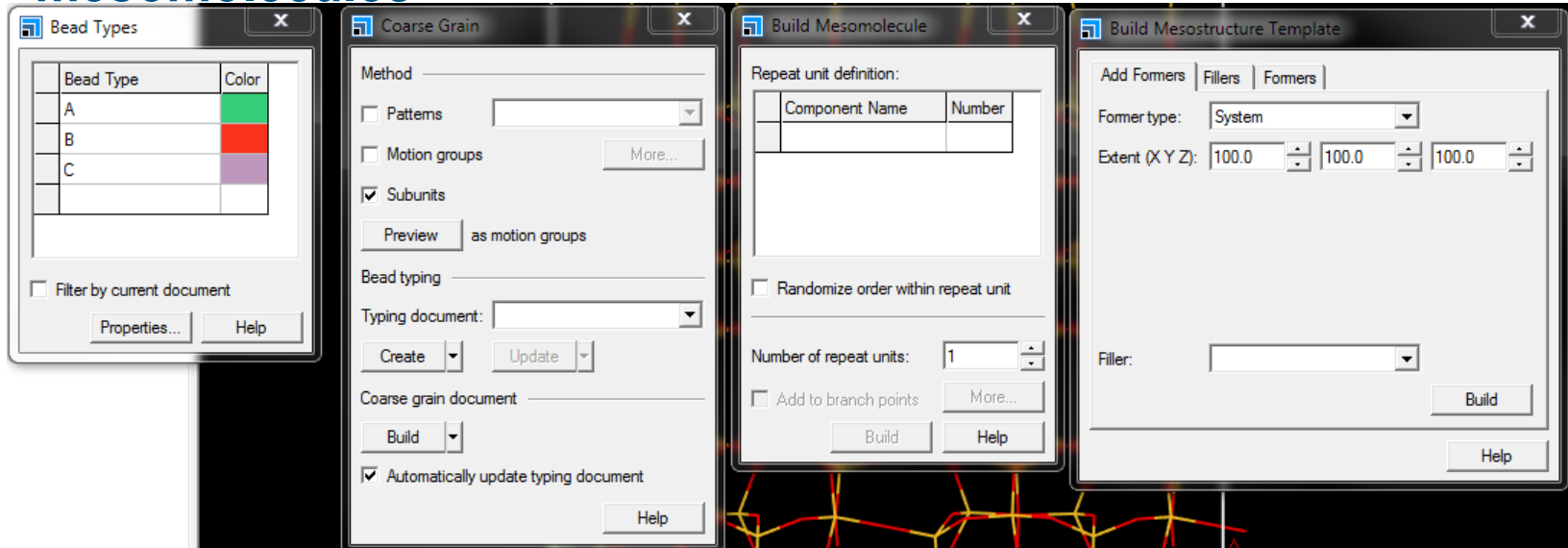
- General Utility Lattice Program (GULP) Support for 3D periodic solids, gas phase clusters, and isolated defects in bulk materials
- EAM potentials and Shell models, ReaxFF and many more system specific potentials supported
- Calculate phonon DOS and EFG tensor
- Fit forcefield parameters using user interface



Prof. Julian Gale <https://nanochemistry.curtin.edu.au/gulp/news.cfm>

Calculations – Mesoscale

MS Mesocite Builder: UI makes it easy to construct and parametrize mesomolecules



Define Beads/Potential → Construct Mesomolecule → Pack into template → Execute Job

Calculations – Mesoscale

MS Mesocite ForceFields

- Martini and Shinoda FF supported

Coarse Graining using Martini Bead types

(P) Polar

(N) Non-polar

(C) Apolar

(Q) Charged

(S) for rings

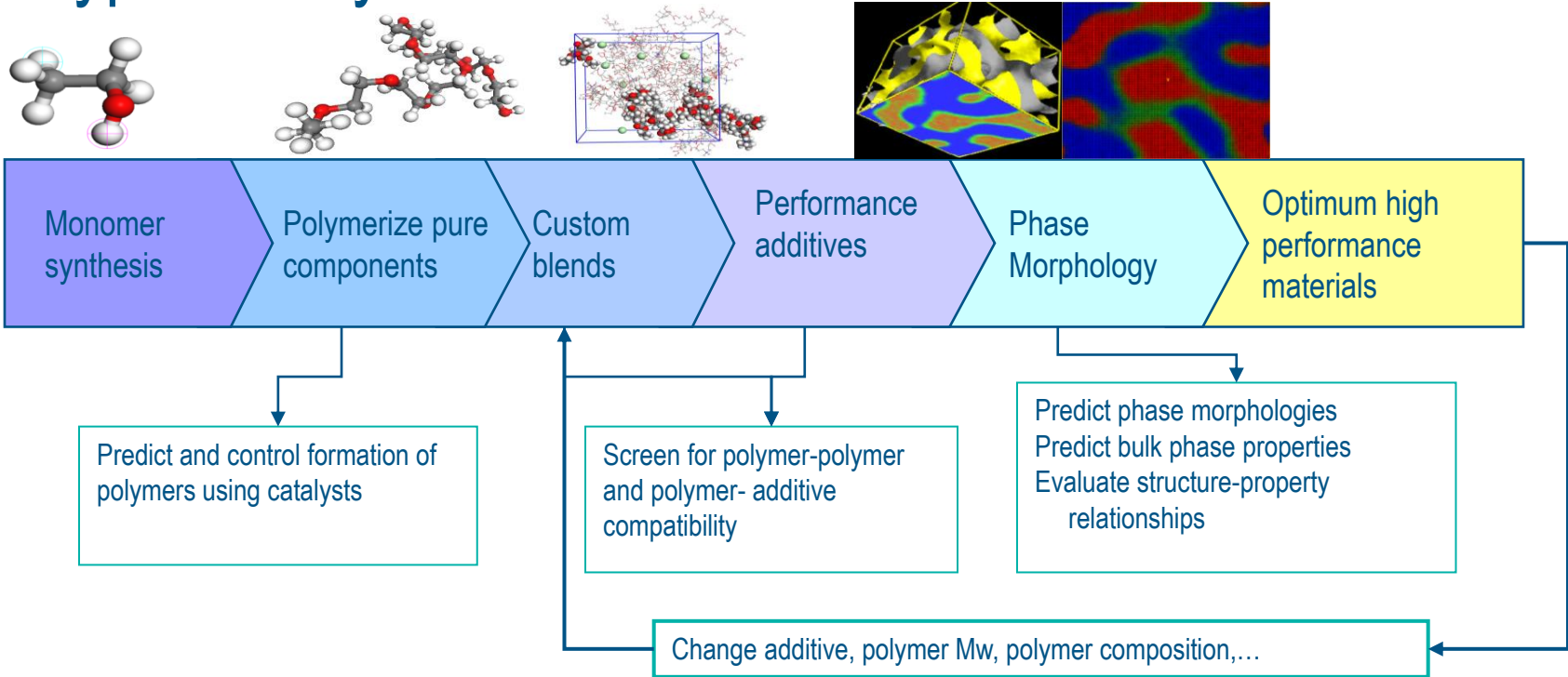
TABLE 1: Interaction Matrix^a

sub	Q					P					N					C				
	da	d	a	0	5	4	3	2	1	da	d	a	0	5	4	3	2	1		
Q	da	O	O	O	II	O	O	O	I	I	I	I	IV	V	VI	VII	IX	IX		
	d	O	I	O	II	O	O	O	I	I	I	III	IV	V	VI	VII	IX	IX		
	a	O	O	I	II	O	O	O	I	I	I	III	IV	V	VI	VII	IX	IX		
	0	II	II	II	IV	I	O	I	II	III	III	III	IV	V	VI	VII	IX	IX		
	5	O	O	O	I	O	O	O	O	I	I	I	IV	V	VI	VI	VII	VIII		
P	4	O	O	O	O	I	I	II	III	III	III	III	IV	V	VI	VI	VII	VIII		
	3	O	O	O	I	O	I	I	II	II	II	II	IV	IV	V	V	VI	VII		
	2	I	I	I	II	O	II	II	II	II	II	II	III	IV	IV	V	VI	VII		
	1	I	I	I	III	O	II	II	II	II	II	II	III	IV	IV	IV	V	VI		
	da	I	I	I	III	I	III	II	II	II	II	II	IV	IV	V	VI	VI	VI		
N	d	I	III	I	III	I	III	II	II	II	III	II	IV	V	VI	VI	VI	VI		
	a	I	I	III	III	I	III	II	II	II	II	III	IV	IV	V	VI	VI	VI		
	0	IV	IV	IV	IV	IV	IV	III	III	IV	IV	IV	IV	IV	IV	IV	V	VI		
	5	V	V	V	V	V	V	IV	IV	IV	IV	IV	IV	IV	IV	IV	V	V		
	4	VI	VI	VI	VI	VI	VI	V	IV	IV	V	V	V	IV	IV	IV	V	V		
C	3	VII	VII	VII	VII	VI	VI	V	V	IV	VI	VI	IV	IV	IV	IV	IV	IV		
	2	IX	IX	IX	IX	VII	VII	VI	VI	V	VI	VI	V	V	V	IV	IV	IV		
	1	IX	IX	IX	IX	VIII	VIII	VII	VII	VI	VI	VI	VI	V	V	IV	IV	IV		

^a Level of interaction indicates the well depth in the LJ potential: O, $\epsilon = 5.6$ kJ/mol; I, $\epsilon = 5.0$ kJ/mol; II, $\epsilon = 4.5$ kJ/mol; III, $\epsilon = 4.0$ kJ/mol; IV, $\epsilon = 3.5$ kJ/mol; V, $\epsilon = 3.1$ kJ/mol; VI, $\epsilon = 2.7$ kJ/mol; VII, $\epsilon = 2.3$ kJ/mol; VIII, $\epsilon = 2.0$ kJ/mol; IX, $\epsilon = 2.0$ kJ/mol. The LJ parameter = 0.47 nm for all interaction levels except level IX for which $\sigma = 0.62$ nm. Four different CG sites are considered: charged (Q), polar (P), nonpolar (N), and apolar (C). Subscripts are used to further distinguish groups with different chemical nature: 0, no hydrogen-bonding capabilities at present; d, groups acting as hydrogen bond donor; a, groups acting as hydrogen bond acceptor; da, groups with both donor and acceptor options; 1–5, indicating increasing polar affinity.

The MARTINI forcefield: coarse grained model for biomolecular simulations, J. Phys. Chem. B, 111:7812-7824, 2007

Typical Polymer Workflow



Can also predict mechanical properties, diffusion, surface binding energies,...

Calculations – Quantum Chemistry

Quantum Chemistry

MS DMOL3

- Workhorse Density functional theory quantum chemistry program
- Based on Numerical Atomic Orbitals for basis functions
- Support for latest functionals
- Performs gas and solution phase periodic DFT calculations for crystals and molecules

ΔH_F , ΔG_F , ΔE_A , ΔS , K_R
Catalyst Design and
Reaction Kinetics
Cracking, Polymerization,
Heterogeneous catalysis,
Reaction rate calculation

DFT for molecules and solids
MS DMOL3
MS DMOL3 Solid State

Calculations – Quantum Chemistry

Quantum Chemistry

MS DMOL3

- Transition state search, implemented NEBM (LST, QST, HL)
- Solvent effects incorporated via SCRF method. Support for COSMO model
- Dispersion corrections via TS, OBS, Grimme
- Optical property calculation via TD-DFT
- Band structure, DOS supported

ΔH_F , ΔG_F , ΔE_A , ΔS , K_R

Catalyst Design and
Reaction Kinetics

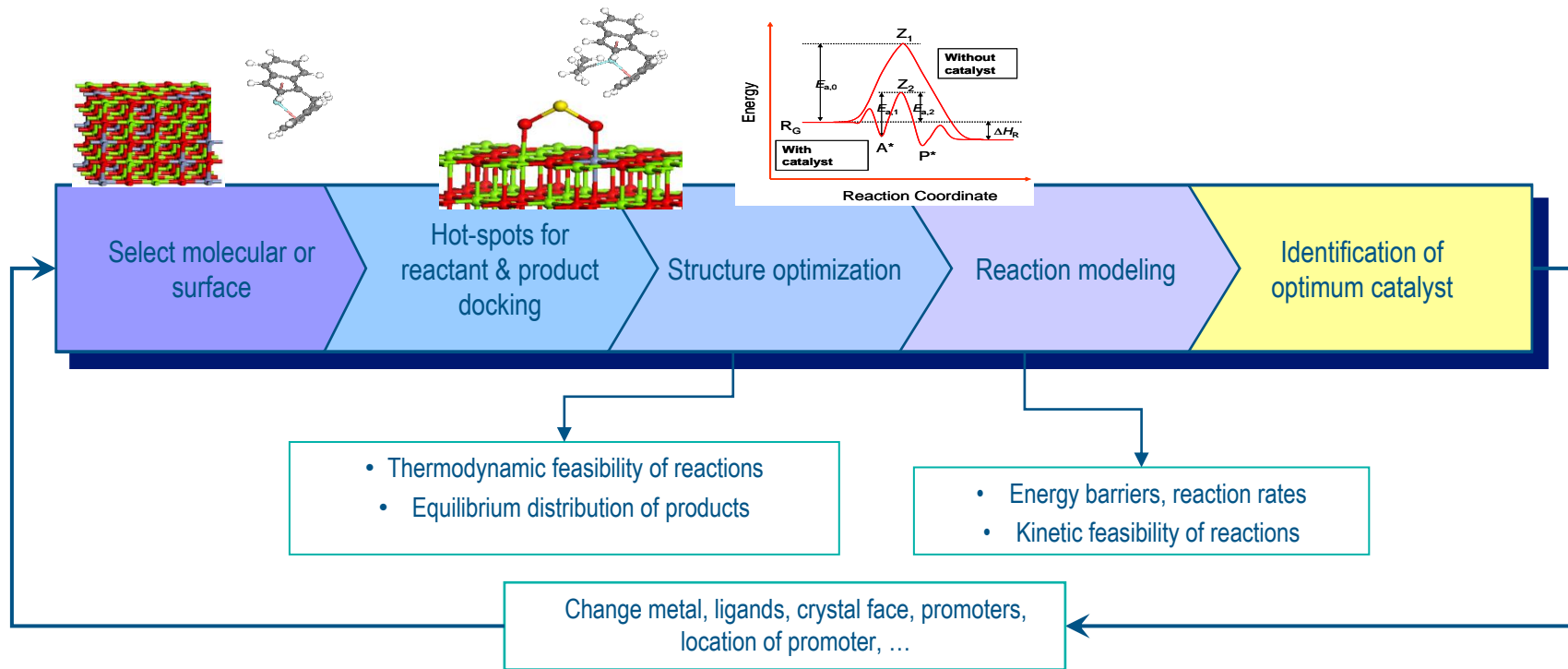
Cracking, Polymerization,
Heterogeneous catalysis,
Reaction rate calculation

DFT for molecules and solids

MS DMOL3

MS DMOL3 Solid State

Catalysis Workflow



Homogeneous Catalysis

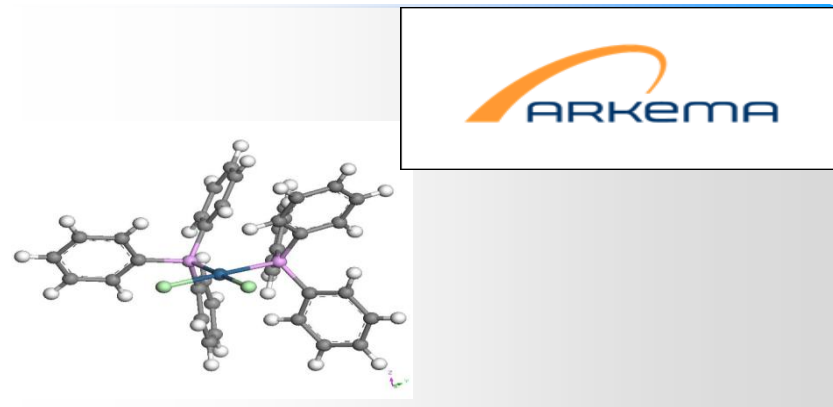
Polymerization can be done using homogeneous catalysts – DOW Chemicals

Problem

- Select ligands to achieve target reactivity
- Ligand synthesis and x-ray experiments are costly and lengthy.
- Standard selection criteria not applicable (too many substituent etc)
- Need a method that is quick and easy to run by non-experts
- QSAR good but not necessarily predictive

Solution

- Predict ligand properties before synthesis
- Build reaction specific QSAR models for key property: coupling constant.



Result

- High quality model obtained.
- Descriptors in models have understandable meaning.
- Accessible with simple computational methods.

Lanthanide Catalysts using DMol3

- La_2O_3 , LaOCl , LaCl_3 used in commercial reactions,
 - Production of vinyl chloride, alkane conversion to chloride
- Studied model reaction of
 - $\text{CCl}_4 + 2 \text{H}_2\text{O} \rightarrow \text{CO}_2 + 4 \text{HCl}$
 - A collaboration between Dow Chemical and several Universities
- Use experiment & theory to link surface properties with catalytic activity
- Detailed work from can be found in



JPC:B 108 (2004) 15770; *Chem. Euro. J 10* (2004) 1637; *JPC:B 109* (2005) 11634

Calculations – Quantum Physics

MS CASTEP

- DFT Plane-wave pseudopotential code for solids state materials
- Developed by the Castep Development Group, Cambridge
- Support for both UltraSoft and Norm Conserving pseudopotentials
- LDA(+U), GGA, B3LYP, HSE03/06 supported
- Dispersion corrections via TS, OBS, Grimme

Quantum Physics

ΔH_F , ΔG_F , ΔE_A , ΔS , K_R
Reaction Kinetics
Heterogeneous catalysis
e-Ph coupling
RAMAN and IR
Solid-State NMR

DFT for solids
MS CASTEP
MS CASTEP NMR

Calculations – Quantum Physics

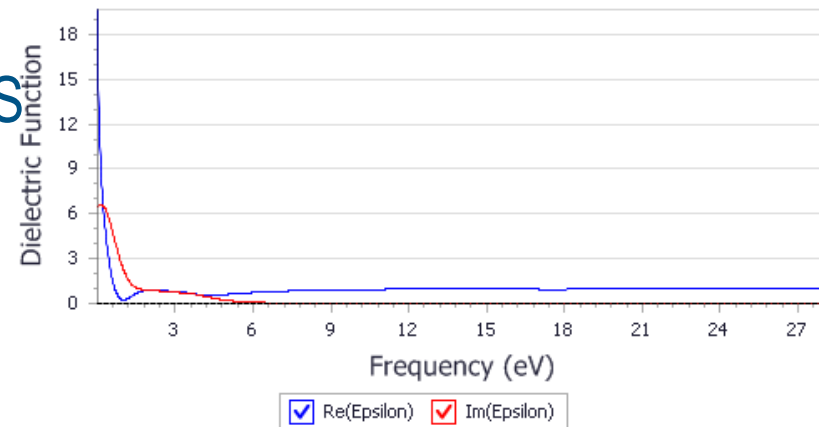
MS CASTEP

- Molecular Dynamics
- Elastic Constants
- PDOS, LDOS and Band structures
- Electron-Phonon coupling, Phonon DOS
- Electron Localization Function
- Core level spectroscopy
- IR, Raman Spectra, STM profiles
- Solid-State NMR predictions

CASTEP Optical Properties

Scissors operator= 0 eV, Instrumental smearing : 0.5 eV

Calculation geometry: Polarized, polarization direction: (1.000 0.000 0.000)



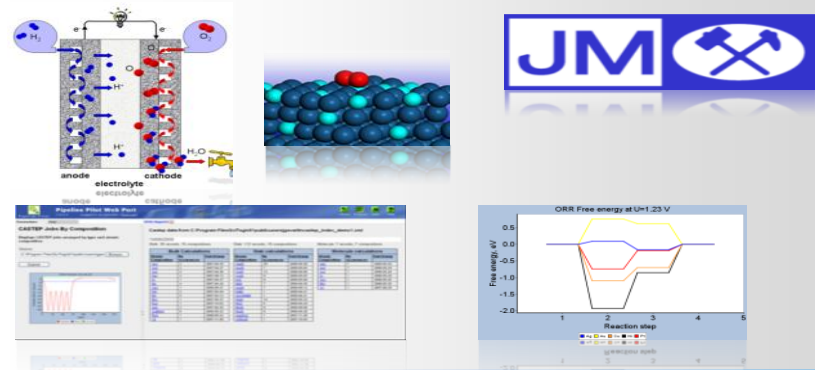
Heterogeneous Catalysts

Problem

- Develop fuel cells as an affordable “green” energy solution.
- Replace expensive platinum while maintaining high performance.
- Find the “best” material among 1000s, on schedule and in budget.

Solution

- Utilize predictive analytics to speed candidate material assessment.
- Create reporting system for collaborative decision making.
- Database to capture computational results
- Highly automated workflow system



Result

- Developed efficient, reusable application for discovery and optimization of fuel cell materials.
- Identified lead material with lower cost than pure Pt.
- Screened 2000+ structures with zero experimental cost.
- Database has become a knowledge base

Solid state NMR

Function

Predicts key magnetic resonance properties of molecules and solid state materials

Theory

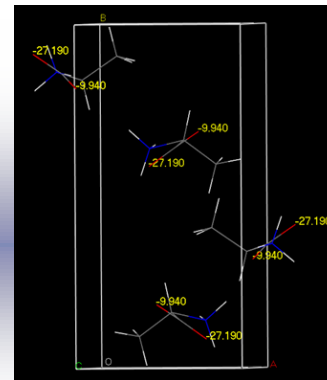
- Based on the CASTEP density functional theory (DFT) program
- Uses the gauge-including projector augmented-wave (GIPAW) approach
- Includes relativistic effects

Key Properties

- NMR chemical shift tensor
- Isotropic shifts
- electric field gradient tensors
- Visualization of isotropic shifts and electric field gradients
- **Very Accurate!**

Parameter	Theory	Expt
σ_{iso} O1	-27.19	
δ_{iso} O1	294.49	284
σ_{iso} O2	-9.94	
δ_{iso} O2	277.24	260.5
C_q O1	8.29	7.86
C_q O2	6.78	6.53
η_Q	0.26	0.28
η_Q	0.65	0.70

$$\delta_{\text{iso}} = \sigma_{\text{reference}} - \sigma_{\text{observed}}$$



Assignment of ^{17}O shifts in L-Alanine

Materials

Molecules, solids, interfaces and surfaces for a wide range of materials classes including organic molecules, ceramics, and semiconductors.

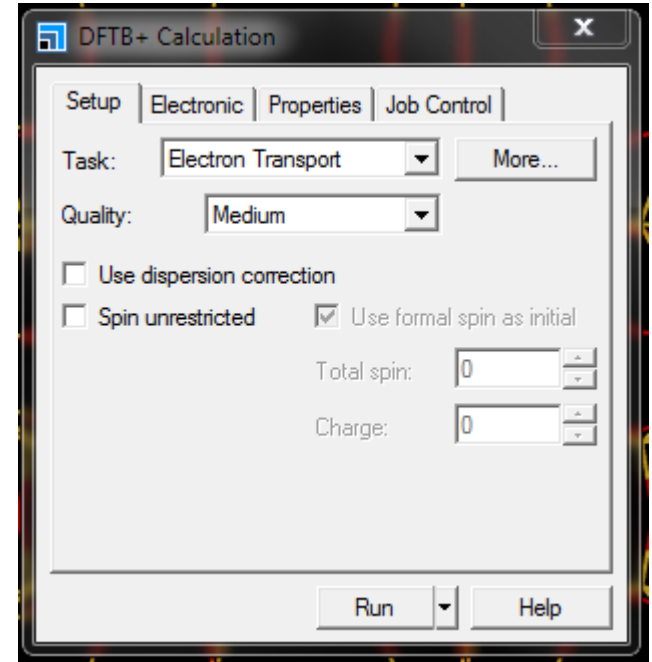
Typical Applications

- perform assignment of the observed NMR spectra
- assign chemical shifts to atoms unambiguously
- discriminate between crystal polymorphs

Calculations – Quantum Physics

MS DFTB+

- Based on the tight-binding ansatz, “like” LCAO principle
- Enables calculations over larger number of atoms
- Uses Slater-Kosher PP libraries
- Offers similar functionality as CASTEP to a limited set of atoms
- Electron transport



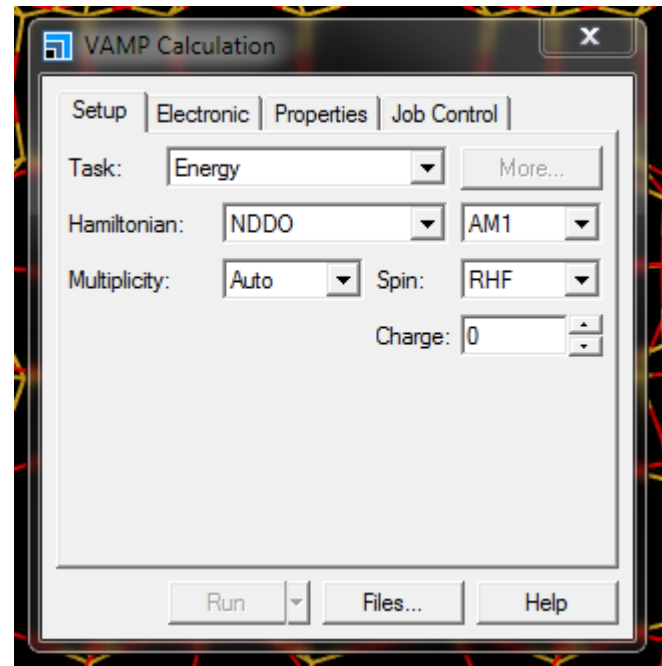
Prof. Thomas Frauenheim
Bremen Center for Computational Materials Science

Calculations – Semi-Empirical

MS VAMP - Vectorized AMPAC (AM1)

- ZDO - Zero differential overlap method
- NDDO (MNDO, AM1, PM3, PM6)
- ZINDO (INDO, CNDO)
- Supports larger system size
- Transition States and H_f
- UV-VIS
- IR
- Orbitals

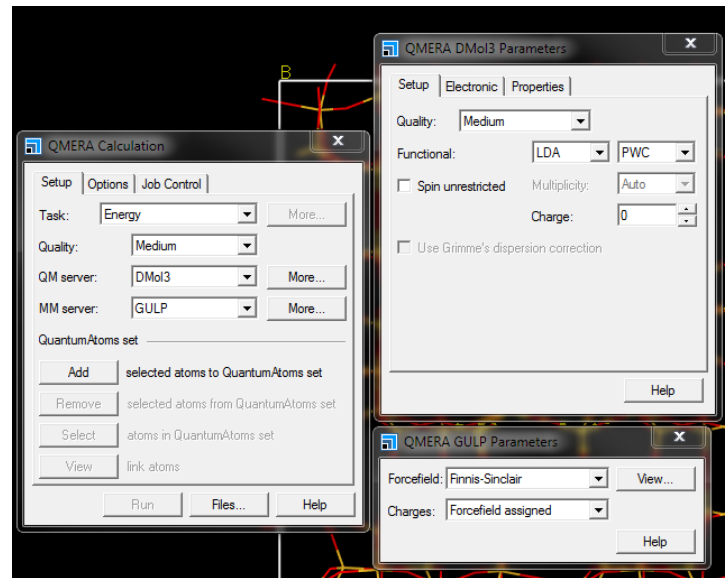
Clark, T.; Alex, A.; Beck, B.; Burkhardt, F.; Chandrasekhar, J.; Gedeck, P.; Horn, A.; Hutter, M.; Martin, B.; Rauhut, G.; Sauer, W.; Schindler, T.; Steinke, T.; Universität Erlangen 2001.



Calculations – QM-MM

MS QMERA

- QMERA offers an accurate way of modelling reactivity at a low computational cost
- QMERA has been tested against other *ab initio* and QM/MM approaches
- QMERA has several embedding schemes: QM-Pot/ONIOM-like and electrostatic additive
- **QMERA is easy to use thanks to MS UI**



DMol³ for DFT
GULP for MM

Calculations – QM-MM

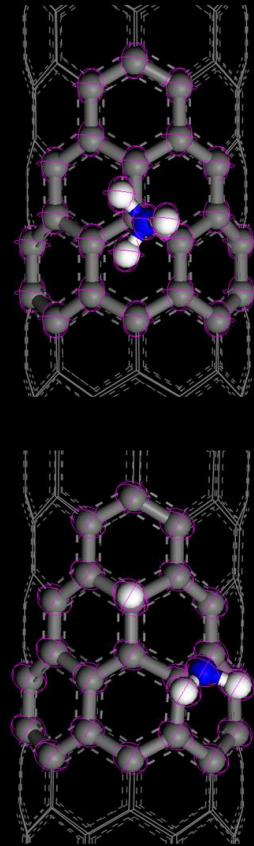
MS QMERA

- combined quantum mechanical (QM) and molecular mechanics (MM)
- Do an MM calculation on whole system (S) – exclude link atoms
- Use QM on the central region C = I + L
- Use MM on the central region C = I + L

$$E_{\text{tot}}^{\text{sub}} = E_{\text{MM}}(S) + E_{\text{QM}}(C) - E_{\text{MM}}(C)$$

Note: requires to have proper forcefield atom types for both the full system S and the inner system C!

Nanotube Based Gas Sensors – Role of structural defects
Chem. Phys. Lett. 2006, **421**, 58



pure-CNT

Calculations – QM-MM

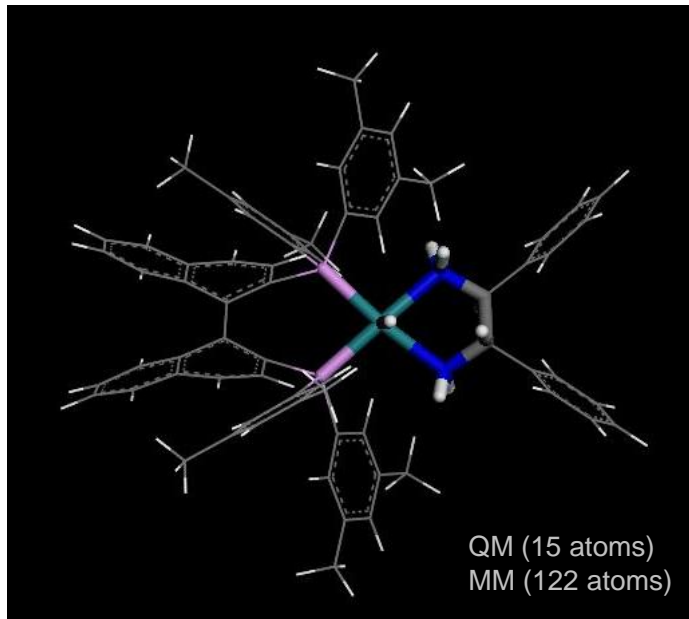
MS QMERA Example

Geometry Optimization of $\text{Ru}(\text{H})_2(\text{diphosphine})(\text{diamine})$ homogeneous catalyst

“New insights into the
enantioselectivity in the hydrogenation
of prochiral ketones”

Samuel A. French, Devis Di
Tommaso, Antonio Zanotti-Gerosa, Fred
Hancock and C. Richard A. Catlow

Chem. Commun., 2007, 2381



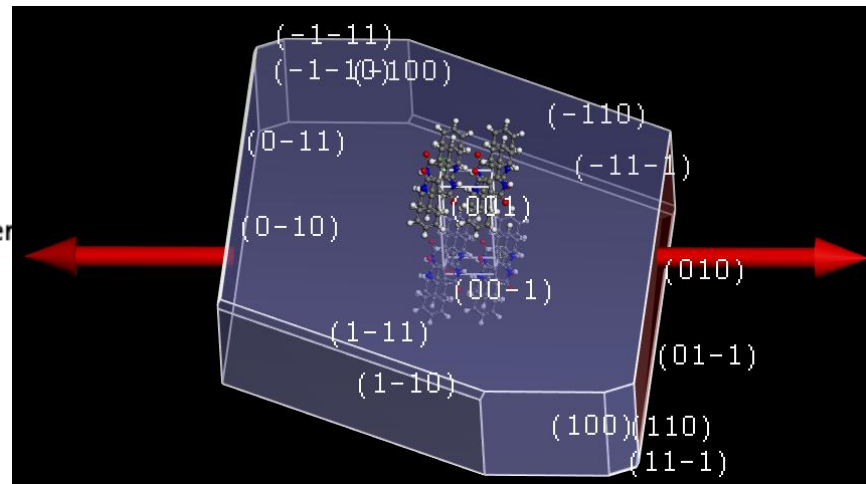
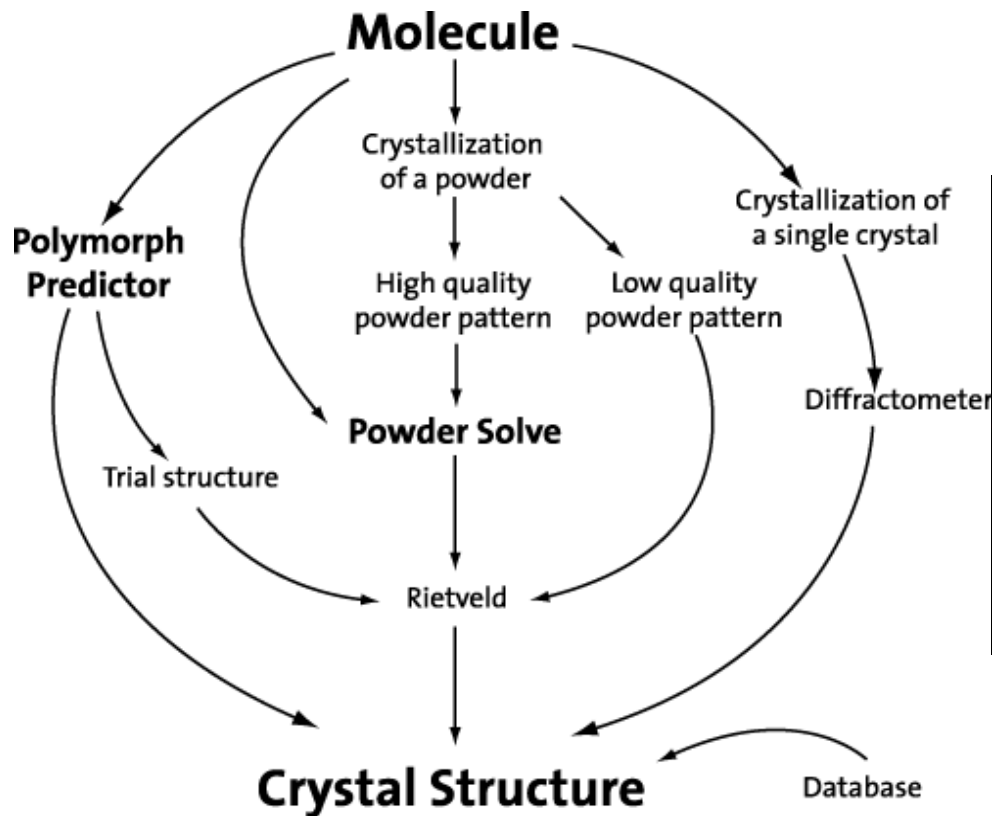
PBE/DND / Dreiding

Electronic additive embedding:
QM region polarized by MM point
charges

ESP charges for MM region

QMERA faster than
DMol³ pure!

MS CRYSTAL Tools

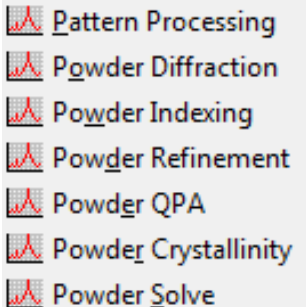


Crystal Morphology of Pigment Red Showing (001) surface to be most stable

MS CRYSTAL Tools

MS Reflex and Reflex Plus

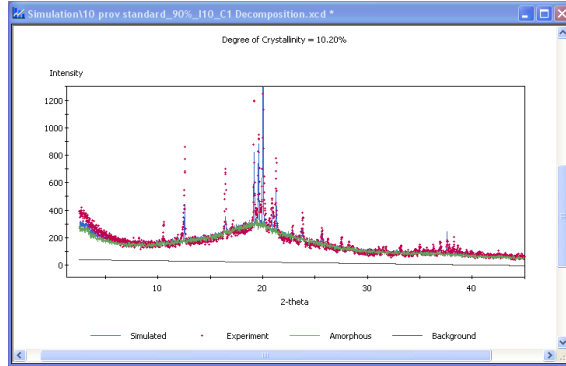
- Comprehensive X-RAY, Neutron, Electron structure solution and Simulation Package
- Indexing (DICVOL91, TREOR90, ITO15, X-Cell [MS Exclusive])
- Refining Powder Diffraction and Structure (Pawely, Rietveld, Pareto)
- Space Group Determination (Figure of Merit Ranking)
- Compare and Refine with experimental patterns
- Account for line broadening, Asymmetry, Line Shift in experimental patterns
- Structure optimization methods using MS QUANTUM AND MS CLASSICAL
- Calculate degree of crystallinity



- Pattern Processing
- Powder Diffraction
- Powder Indexing
- Powder Refinement
- Powder QPA
- Powder Crystallinity
- Powder Solve

Save Settings...

Analytical: Powder Crystallinity



The figure is a screenshot of the "Reflex Powder Crystallinity" software interface. The window title is "Reflex Powder Crystallinity". The "Setup" tab is selected, and the "Diffractometer" sub-tab is active. The "Task" is set to "Phase analysis". The "Crystalline reference" is set to "1 prov indexing_1h30_". The "Amorphous reference" is set to "2 prov_x1_lactose_ar". There is a checkbox for "Use custom range" which is currently unchecked. The "Start" value is 10.0 and the "End" value is 44.0. At the bottom, there are "Calculate" and "Help (Topic?)" buttons.

Powder Crystallinity (MS Reflex) allows users to quantify the amorphous content within a sample.

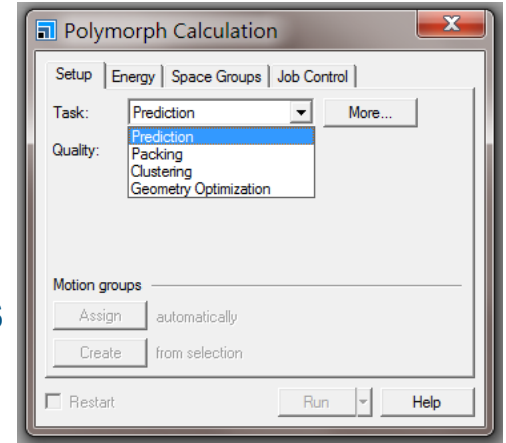
This is often critical because:

- Benchmark measure for efficiency of crystallization process
- Amorphous content can crystallize into different polymorphic forms
- Amorphous content typically shows different dissolution behavior than crystal phase. This can affect bioavailability

MS CRYSTAL Tools

MS Polymorph

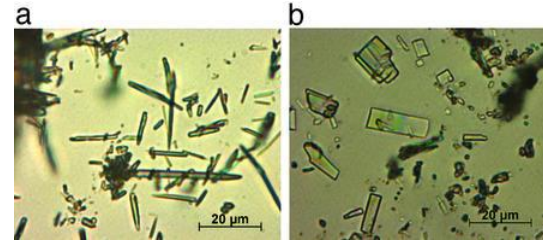
- Predict potential stable or metastable crystal structures of a given compound directly from the molecular structure
- Generate possible packing arrangements in all reasonable space groups - Monte Carlo Simulated Annealing
- Ab initio prediction of polymorphs when experimental powder data is not available
- Predict space group occurrences/population



Exploration of Polymorphic Landscape

Critical Challenges

- Once a potential form is discovered, the risk of polymorphic transformations needs to be assessed
- Unknown polymorphs can cause huge costs, with FDA and patent rights implications



Novir: A famous example of a pharmaceutical polymorph causing huge costs due to its late discovery

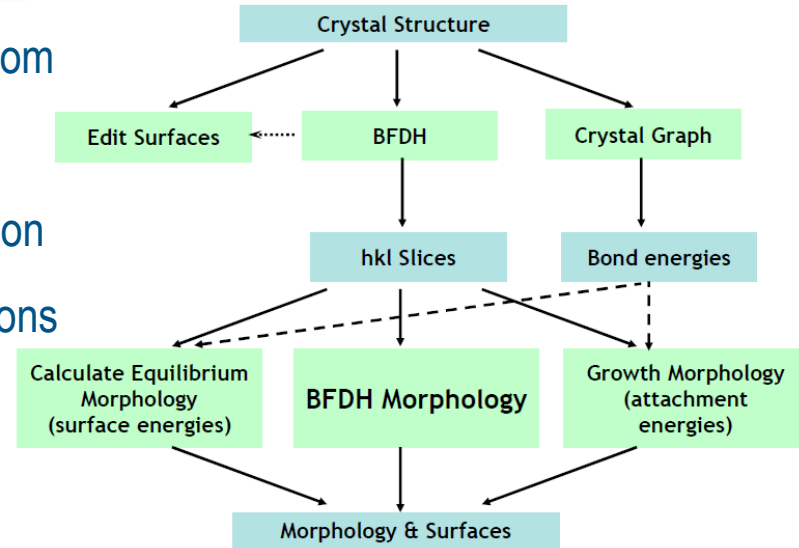
Solutions

- MS Polymorph – a “fast” tool to screen potential packing arrangements
- MS ConQuest – Integration with CCDC’s DB of known crystal structures
- MS Motif – Analysis and statistical scoring of bonding relative to known structures

MS CRYSTAL Tools

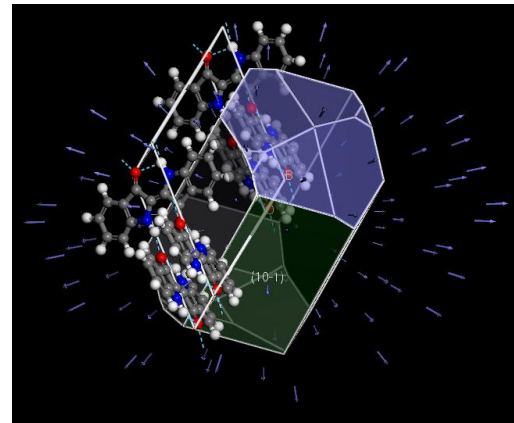
MS Morphology

- De Wulff constructor - Predict external morphology from internal crystal structure
- Bravais-Friedel Donnay-Harker growth plane prediction
- Growth morphology via Attachment Energy Calculations
- Prediction of Equilibrium morphology
- Crystal graph functionality via Periodic Bond Chains

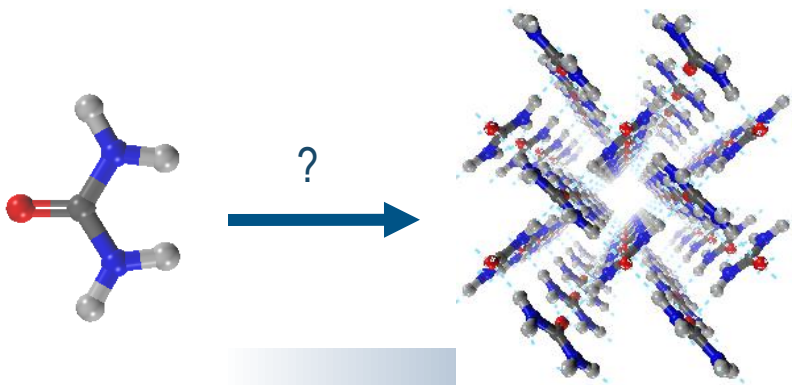


Crystal Morphology

- Estimate relative growth rates of crystal faces to construct crystal morphology.
- MS Morphology allows to predict crystal morphology in vacuum from the atomic structure of a crystal

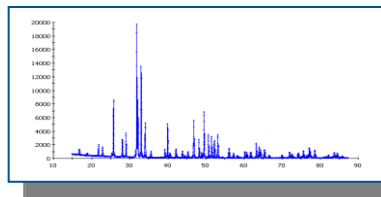


Wulff plot of Indigo Morphology



Characterization of Crystal Workflow

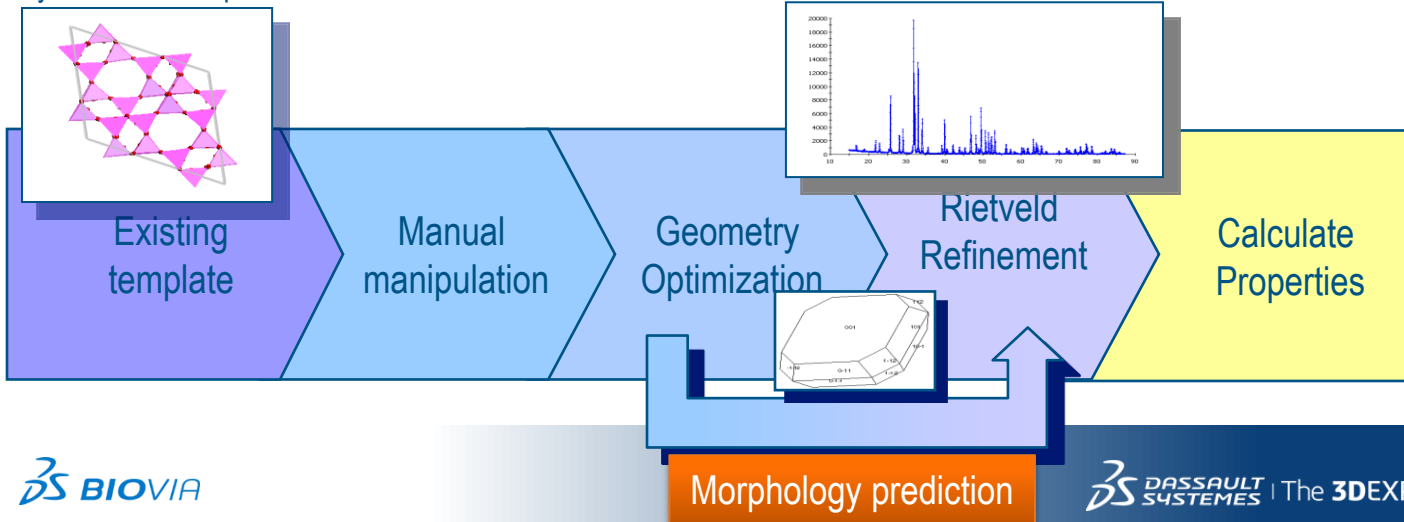
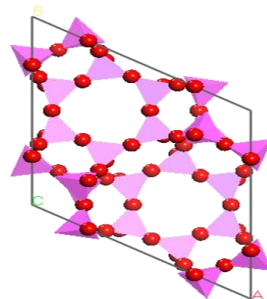
- New crystals with no prior structural information determination with powder diffraction data - Structure
- New crystals with no prior structural information – In-silico structure prediction - Polymorph prediction
- New crystal with some prior structural information



- Indexing
- Pawley refinement
- Structure solution
- Rietveld Refinement



- Polymorph prediction

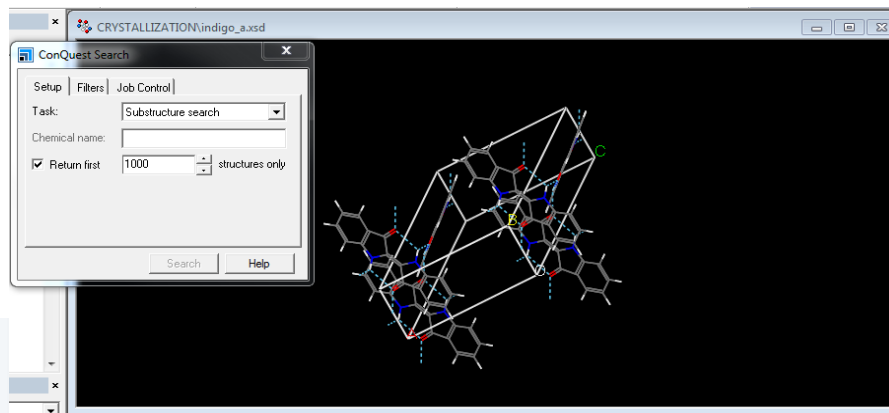


Materials Studio and the CCDC



Cambridge Crystallographic Data Centre

- Connection to Cambridge Structural Database (CSD)
 - information sharing between Materials Studio and **Conquest** from the Cambridge Crystallographic Data Center (CCDC).
 - Ability to transfer substructures from MS to CSD query engine
 - Ability to import CSD query results for further analysis
- Motif Search
 - analyse hydrogen bond motifs formed between particular functional groups in a crystal structure

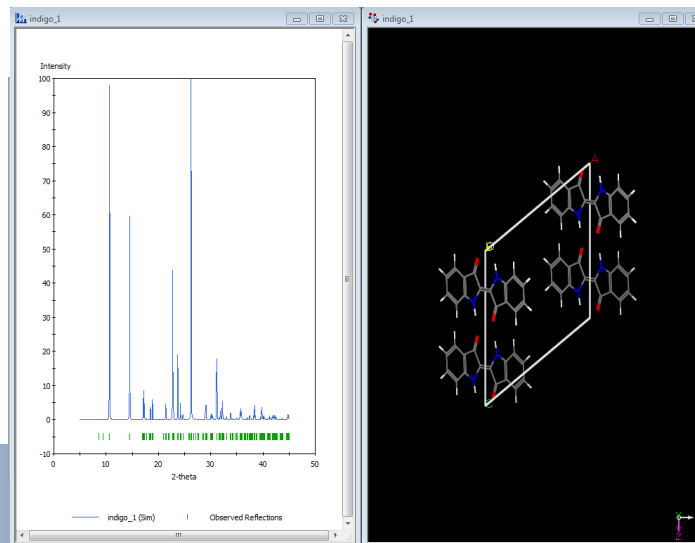
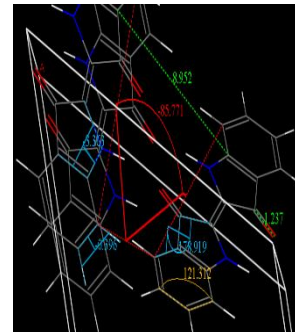
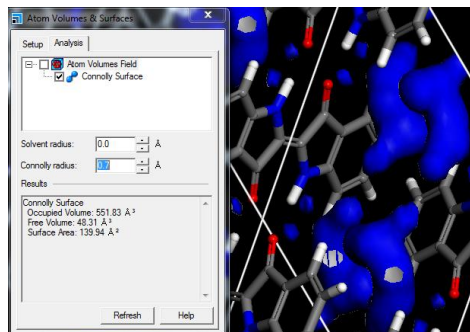


Crystal visualization & properties

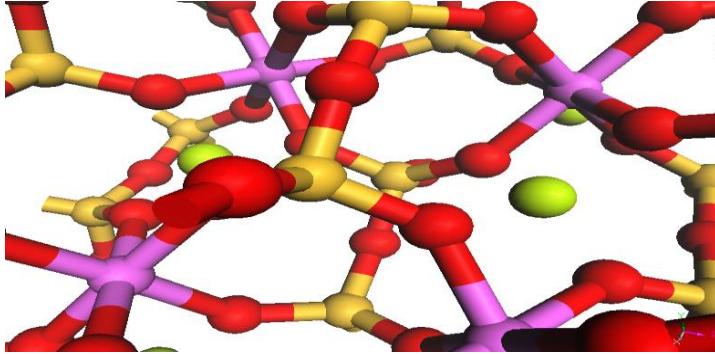
Crystals Properties

- Atom volumes & Surfaces
- Simulation of XRPD (Reflex)
- Property Explorer
 - ✓ Density
 - ✓ Unit cell parameters, etc.

Property	Value
AngleAlpha	90.0000
AngleBeta	130.020
AngleGamma	90.0000
BravaisLattice	Primitive Monoclinic
CellVolume	600.134
CenteringType	3D Primitive-Centered
Color	RGB(255, 255, 255)
GroupName	P21
IsVisible	Yes
LatticeOrigin	(0.000000, 0.000000, 0.000000)
LatticeRepresenta...	3D Monoclinic-B
LengthA	10.8400
LengthB	5.88700
LengthC	12.2800
Name	P21
NumOperators	2
OrientationConven...	C along Z, B in YZ plane
SpaceGroupCrysta...	2
SpaceGroupCrysta...	Monoclinic
SpaceGroupITNu...	4
SpaceGroupLau...	2/m(B)
SpaceGroupLong...	P 1 2 1 1
SpaceGroupQualif...	B-Unique
SpaceGroupScho...	C2-2
Style	Solid
SymmetryAxes	x,y,z
VectorA	(8.30149, 1.09059e-015, -6.97072)
VectorA/Velocity	(0.000000, 0.000000, 0.000000)
VectorB	(0.000000, 5.88700, 0.000000)
VectorB/Velocity	(0.000000, 0.000000, 0.000000)
VectorC	(0.000000, 0.000000, 12.2800)
VectorC/Velocity	(0.000000, 0.000000, 0.000000)








Example Project Areas



Delivering Solutions for Real-World Scientific Problems

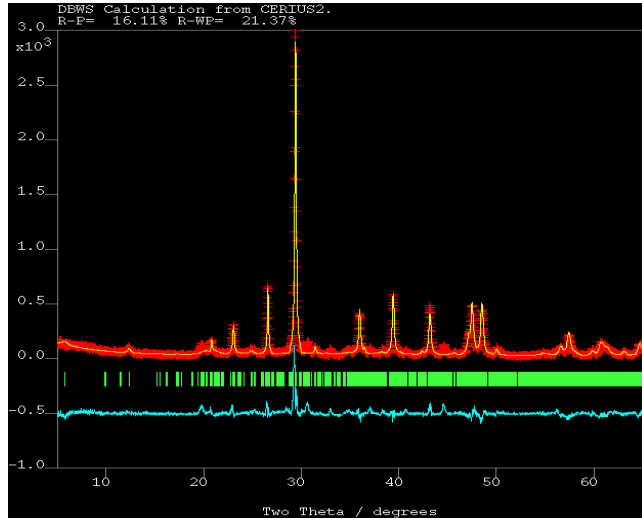
- Statistical Correlations
- Spectral Analysis
- Structural Characterization
- Analysis of Solids
- Analysis of Surfaces
- Analysis at Meso scale Level
- Chemical Reactions

Statistical Correlations

	Structure	Activity [y1]	Apol [x1]	Area [x2]	Dipole [x3]	Energy [x4]	Ft
1.		3.150	1.06E+04	270.566	7.139	133.003	
2.		3.450	9.55E+03	242.417	2.056	100.681	
3.		4.130	1.17E+04	252.990	1.037	103.760	
4.		3.450	1.17E+04	257.214	2.313	109.687	
5.		3.690	8.65E+03	215.372	1.028	90.970	
6.		4.010	1.17E+04	242.563	2.286	93.813	
7.		4.280	1.17E+04	251.587	1.558	100.894	

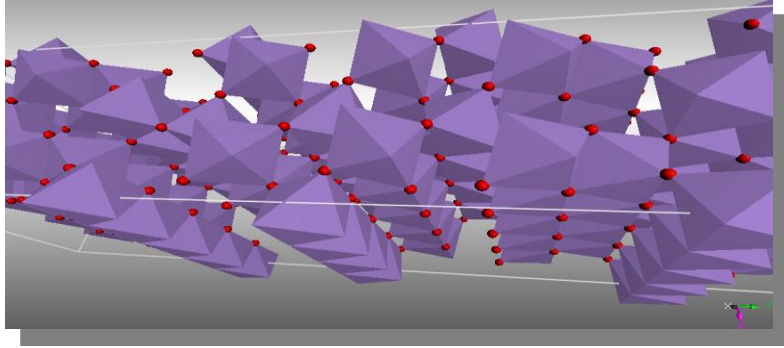
- Optimizing the brilliance of a flare used in the US Army
- A combination of formulation and statistical correlation was used
- Independent variables – concentration of components in the mixture
- Dependent variables – information about the properties of the mixture
- Genetic function algorithm allowed the study of linear, second order and non-linear effects
- Simple interpretable models help design better flares

Spectral Analysis



- A major concern in quantifying types, concentration and composition of minerals in reservoir rocks using XRD is the complexity of the profile due to preferred orientations and structure modifications.
- Computational work at Accelrys involved
 - Clean-up of experimental XRD data
 - Simulation of XRD for various minerals
 - Correction for preferred orientation
 - Geometry optimization of substituted structures
 - Study of the effect of chemical substitution
 - Development of early informatics component to simplify and accelerate the analysis of complex XRD patterns.

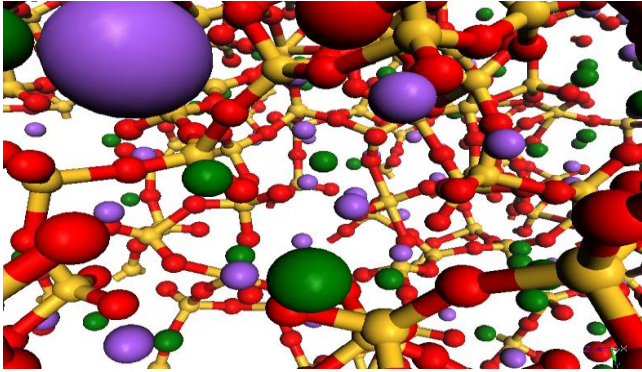
Structural Characterization



J. Solid State Chem. 177, 165 (2004)

- The XRD pattern of γ -MnO₂ (used in batteries) is of a poor quality and varies depending on the production process.
- Computational work at Accelrys showed
 - Particular effects of De Wolff disorder, microtwinning and point defects on XRD patterns.
 - Structural features in CMD and EMD from comparisons of simulated with experimental XRD patterns.
 - De Wolff disorder to be a major factor in determining the structure of γ -MnO₂.
 - CMD materials contain larger percentage of pyrolusite while EMD contain more ramsdellite.
 - EMD is higher in energy than CMD variants.

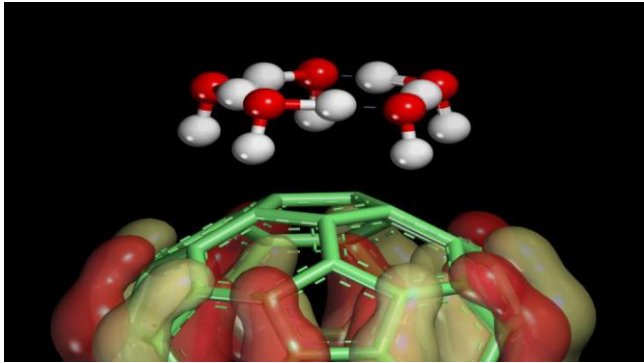
Analysis of Solids



Electronic, Optical, Magnetic,
Vibrational, Thermal, Electrical,
Viscoelastic properties etc.

- A concern in glass fiber production is how to increase resistance to atmospheric moisture while maintaining biodegradability.
- Computational work at Accelrys showed
 - Correlation of glass composition and network density with water reactivity.
 - Sensitivity of cation diffusion in the presence of water.
 - The favorable role of cation on hydrolysis reactions and on the mechanical stress on glass.

Analysis of Surfaces & Interfaces

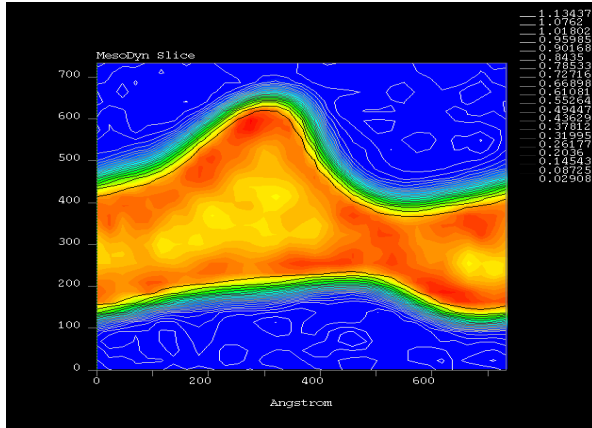


Phys. Rev. Lett. 87, 155502 (2001)

Metals, Alloys, Oxides, Zeolites,
Ceramics, Glass, Minerals,
Semiconductors, Superconductors,
Polymers

- A concern in a field-emission based flat-panel display device is to reduce the operating voltage.
- Experiments at Motorola showed that adsorbed water vapor enhances field-emission current.
- Computational work at Accelrys revealed:
 - The interaction of carbon nanotube and water is weak in zero electric field
 - Under emission conditions, large electric field at the tube tip stabilizes the binding of adsorbate
 - Under emission conditions, large electric field at the tube tip makes it easier to extract electrons through the formation of water clusters leading to a reduction in the Ionization Potential of the nanotube

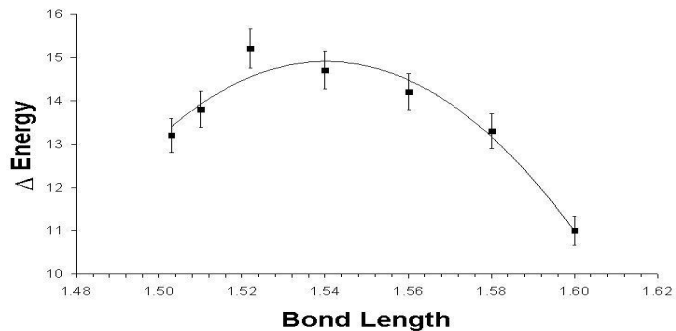
Analysis at the Meso Scale



- A concern is in the production of polymer blends where expensive copolymer compatibilizing agents sometimes phase separate out of the blend.
- Computational work at Accelrys revealed an alternate approach:
 - Grafting one of the blend components with an inexpensive random copolymer
 - This approach results in a strongly mixed interfacial region.
 - This approach increases the adhesion between the phases.

Micelle formation, Colloidal floc building, Rheological properties, Miscibility, Glass transition temperatures, Polymer morphology, Diffusion

Chemical Reactions



Homogenous and
Heterogenous reactions

- A concern in the production of chemicals and polymers is the generation of toxic wastes.
- Computational work at Accelrys
 - Showed the role of the metal catalyst in the formation reaction
 - Revealed the role of solvent in changing the charge state of the metal catalyst
 - Confirmed the reaction mechanism
 - Helped to predict the reaction including solvent effects (proved later to be correct from experiments)
 - Involved the development of informatics component used in statistical correlation to predict reactions

Materials Studio

The screenshot displays the Materials Studio interface with several key components highlighted by callouts:

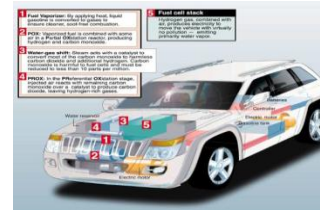
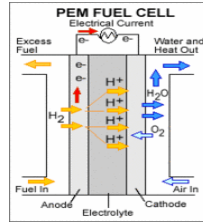
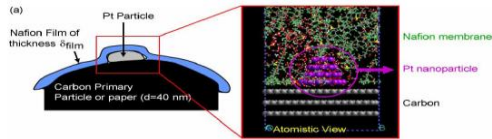
- Tools:** A callout points to the top toolbar containing various modeling and simulation tools.
- Files & Folders:** A callout points to the Project tree on the left, showing a hierarchical view of files and folders such as 'UV spectra' and 'indigo_1 VAMP GeomOpt'.
- Properties:** A callout points to the Properties panel at the bottom left, which shows a table of properties for the selected 'Bond'.
- Figures & Tables:** A callout points to the central workspace, which contains a 'Vamp Optimization Convergence' plot and a 3D ball-and-stick molecular model of indigo.
- Jobs running:** A callout points to the Jobs panel at the bottom, which displays a table of running jobs.

Property	Value
BondOrder	
BondType	
ChemicalType	
IsVisible	Yes
Length	
MidPt	
Name	
SpecialPositionO...	1
Style	Bell and Stick
Construct...	x,y,z
instr...	Identity
privat...	x,y,z
privat...	Identity
multipl...	1

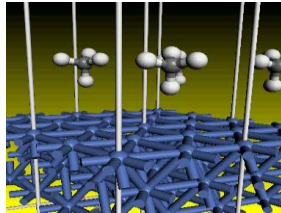
Jobs	Gateway	Server	Status	Progress	Start Time	Results Folder
<input checked="" type="checkbox"/> indigo...	7056N	golf:188...	VAMP	starting		.\indigo\indigo_1 VAMP ...

Chemicals and Materials R&D Process

Automotive (Fuel Cells)



Chemicals (Reactions)



Fundamental
research

Discover

Applied
research

Optimize

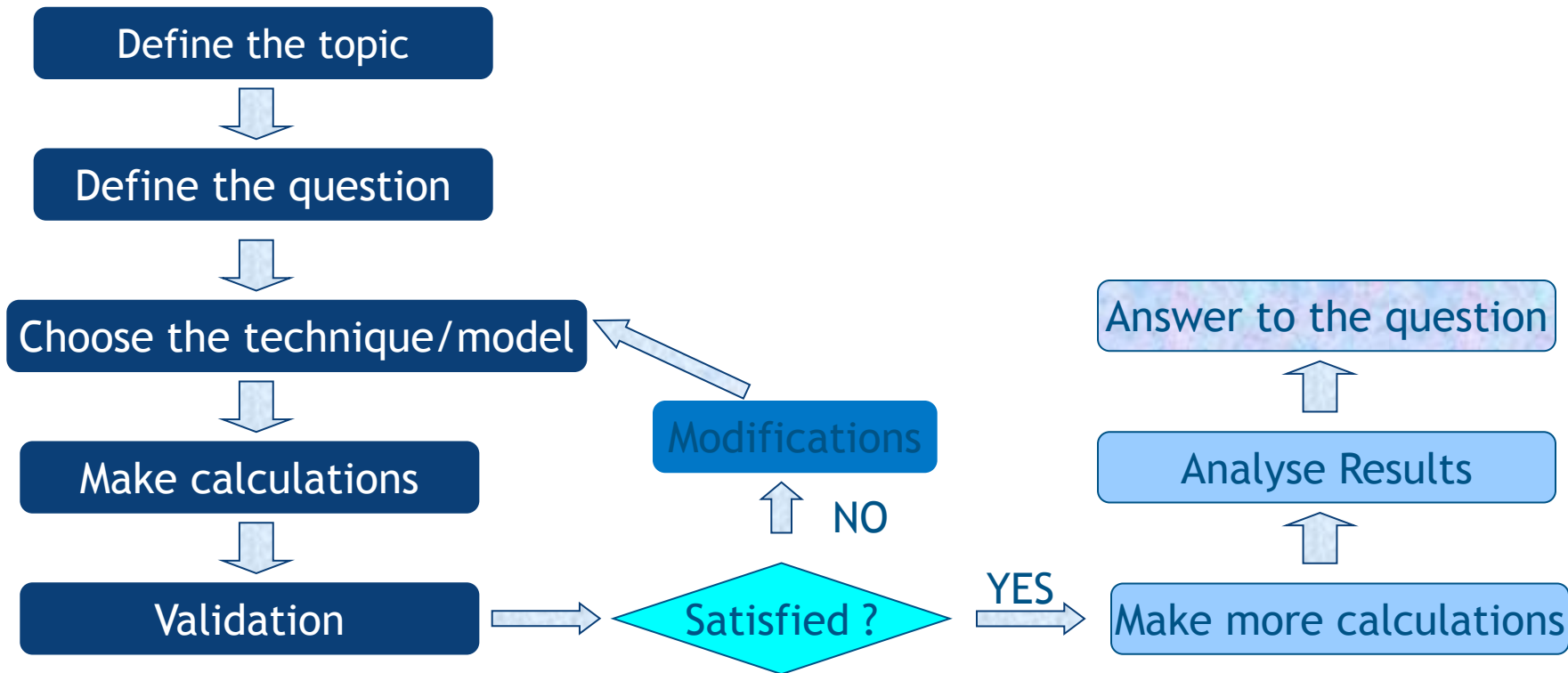
Product
development

Scale-up

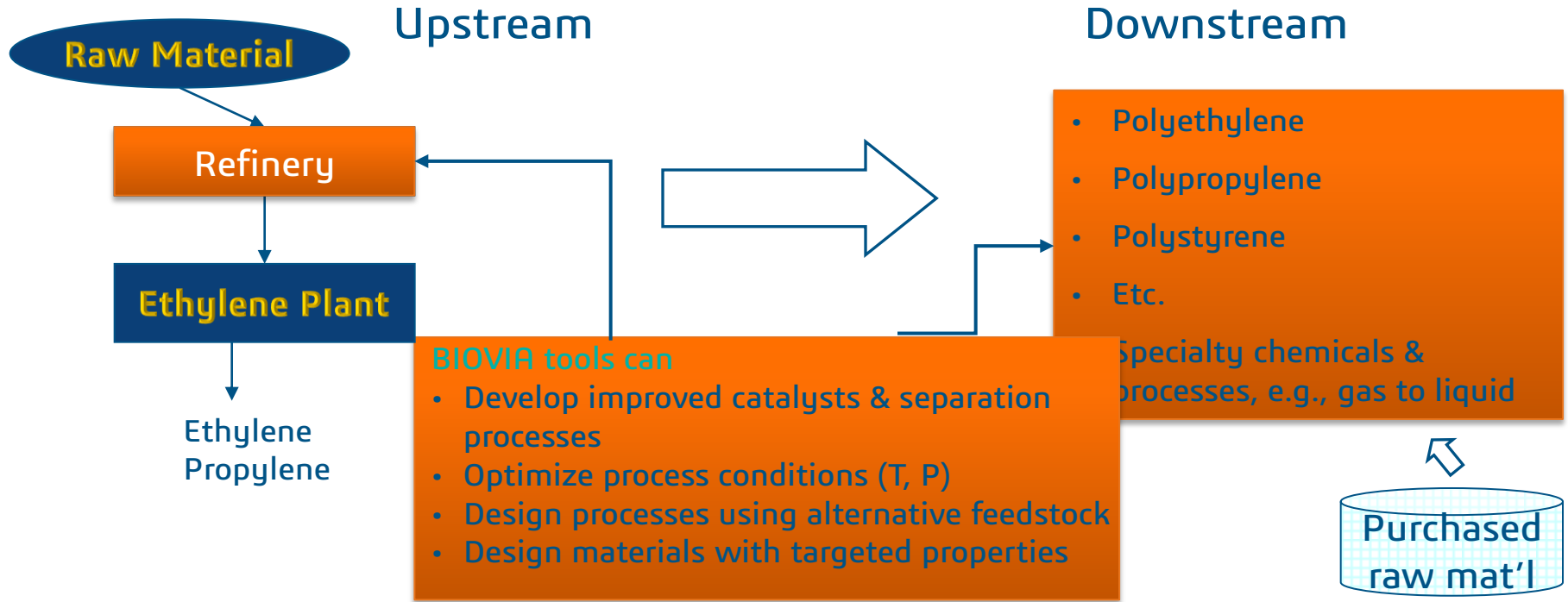
Manufacturing

Pilot

Asking the right questions



Industry Solutions: Oil and Gas



Adapted from Tjoa, Cervantes, Nakagawa, "Optimization based approach for managing enterprise-wide business planning in a petrochemical industry," presented to AIChE 27 April 2004

Industry Solutions: Oil and Gas

Catalysis

Homogenous Catalysis

Downstream Processing
Production of Vinyl chloride,
Alkane conversion to chloride

JPC:B **108** (2004) 15770

Chem. Euro. J **10** (2004) 1637

JPC:B **109** (2005) 11634

Heterogenous Catalysis

Crackers
Polymerization Catalysts

Gavartin, et al., *ECS Transactions*,**25**, 1335(2009)

Thermodynamic modelling

- Reaction Optimization
- Vapour Pressure
- Distillation
- Solvation energies
- Process Chemistry
- Process Engineering

Industry Solutions: Oil and Gas Functionality

Applicable Material Studio Modules

1. MS Visualizer and Collection
2. MS Amorphous Cell
3. MS Adsorption Locator
4. MS Conformer
5. MS Sorption
6. MS Forcite (plus, COMPASS)
7. MS DMOL3
8. MS Castep
9. MS Mesocite (optional)
10. MS Synthia (polymers)
11. MS GULP (optional)
12. MS Blends (Phase diagrams)

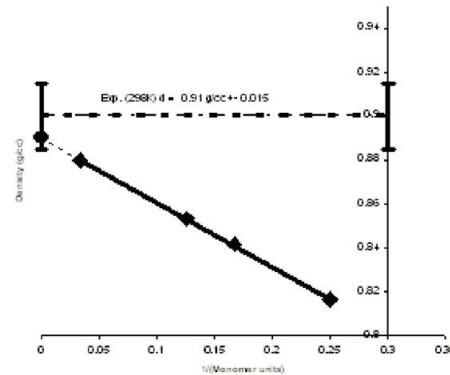
1. 3D Sketch & Build, 3D volume, property and trajectory visualization
2. Preprocess, system construction, packing, etc.
3. Find minimum energy configuration for adsorbed systems
4. Conformational Analysis of molecules
5. Adsorption studies on mesoporous molecules
6. Classical Simulation module for pre-processing or screening of catalytic systems
7. Quantum chemistry simulator for homogenous (downstream conversions) and heterogenous (crackers) systems
8. Quantum Physics simulator for heterogenous systems (crackers)
9. Mesoscale simulations (if polymers are involved)
10. QSAR tools (if polymers are involved)
11. Classical simulation for inorganic solids

Industry Solutions: Consumer and Packed Goods

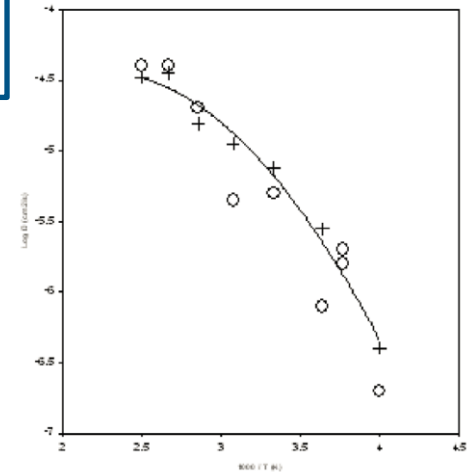
Design of Polymeric Membranes-Modeling and Simulation
Diffusion Studies of Small Gas Molecules in Polymeric Materials

Molecular dynamics (MD) can be accurate enough to predict the self-diffusion coefficient of small gas molecules in amorphous polymeric materials

M. Meunier (BIOVIA Europe)
J. Chem. Phys., **123**, 134906, 2005



Density variation as a function of polymer chain length



Arrhenius plot of the diffusion coefficients of methane and second order polynomial fit

Industry Solutions: Consumer and Packed Goods

Multiscale Modeling Studies of Sulfonated Triblock Copolymers

An important class of thermoplastic elastomers involves polystyrene and polyisobutylene blocks (SIBS). Sulfonated SIBS Triblock Copolymers (S-SIBS) are of particular interest because of potential applications for fuel cell and textile applications, where breathable, protective clothing is required. We have used multiscale modeling to gain an understanding of the static and dynamic properties of these polymer systems at detailed atomistic levels. Quantum chemistry tools were used to elucidate the bonding of water molecules and sulfonate groups. In addition, molecular dynamics was applied to calculate the polymer density at various levels of sulfonation. The structures of polymer with hydronium ions and also water were studied and the mechanism of water self-diffusion was proposed. It was found that with increase of water content the hydronium ions move further away from sulfonate groups. The self-diffusion coefficients of water were found to reproduce well experimental trends. Two different distributions of sulfonate groups were studied: one blocky and another perfectly dispersed. In the case of the blocky architecture, the water clusters are connected at a lower sulfonation level, leading to increased water diffusion coefficients as compared to the dispersed architecture.

“The multiscale simulations allowed us to study microphase separated in composites, fuel cells and other polymeric systems and to predict macroscopic properties at the mesoscale level”

Molecular Simulation, 2006, 32, 163

Jan Andzelm, Ph.D

Computational Chemist

U.S. Army Research Laboratory

Industry Solutions: Consumer and Packed Goods and Polymers

Applicable Material Studio Modules

1. MS Visualizer and Collection
2. Amorphous Cell
3. MS Conformer
4. MS Sorption
5. MS Forcite (plus, COMPASS)
6. MS Mesocite
7. MS Synthia (polymers)
8. MS Blends (phase diagrams)

Functionality

1. 3D Sketch & Build, 3D volume, property and trajectory visualization
2. Preprocess, system construction, packing, etc.
3. Conformational Analysis of molecules
4. Adsorption studies on mesoporous molecules
5. Classical Simulation module for potential development, cross linking reactions, Solubility Parameters. Establish transport phenomenon
6. Mesoscale simulations using forcite developed potentials or native models. Establish transport phenomenon
7. QSAR tools for correlation development

Industry Solutions: HiTech/Semiconductor

Photovoltaics

- Exciton and Trion Dynamics in Bilayer MoS₂,
✓ *Small*, 2015, **11**, 6384
- Tuning the electronic properties of bondings in monolayer MoS₂ through (Au, O) co-doping
✓ *RSC Adv.*, 2015, **5**, 68085
- Electro-optical properties of the perfect reflector material: Poly(3-thiophene boronic acid) semiconducting polymer
✓ *Polym Eng Sci*, 2016, **56**, 707

Semiconductors

- Magnetic MoS₂ pizzas and sandwiches with Mn_n (n = 1–4) cluster toppings and fillings: A first-principles investigation
✓ *Scientific Reports* 2016, **6**, 19504
- Fundamental insights into the electronic structure of zigzag MoS₂ nanoribbons
✓ *Phys. Chem. Chem. Phys.*, 2016, **18**, 4675
- Two-dimensional GeS with tunable electronic properties via external electric field and strain
✓ *Nanotechnology*, 2016, **27**, 274001

Industry Solutions: HiTech/Semiconductor

Applicable Material Studio Modules

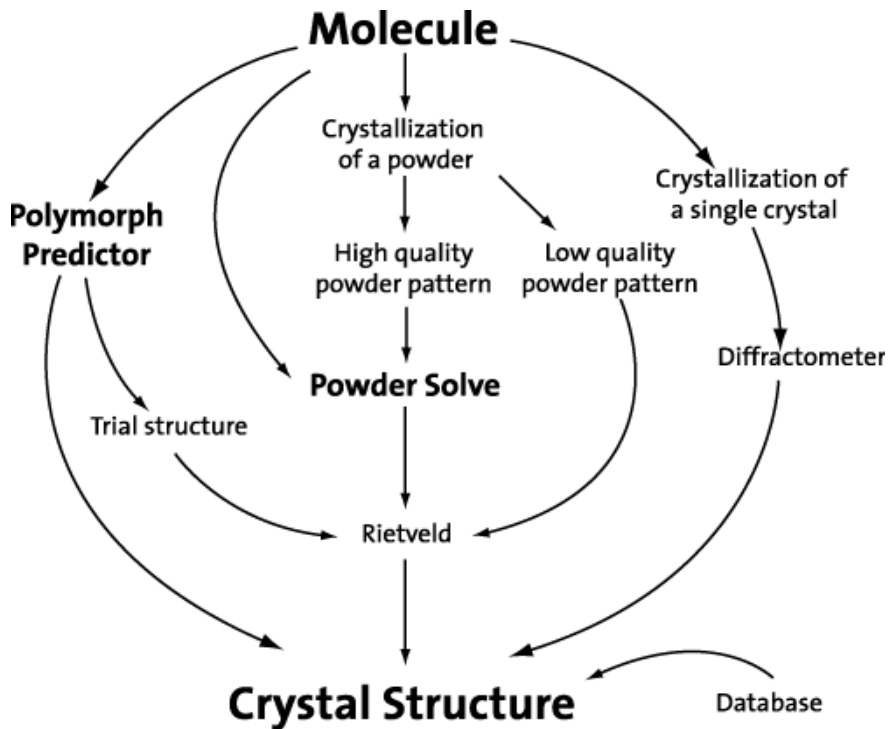
1. MS Visualizer and Collection
2. MS Amorphous Cell
3. MS Adsorption Locator
4. MS Conformer
5. MS Sorption
6. MS Forcite (plus, COMPASS)
7. MS DMOL3
8. MS Castep
9. MS GULP

Functionality

1. 3D Sketch & Build, 3D volume, property and trajectory visualization
2. Preprocess, system construction, packing, etc.
3. Find minimum energy configuration for adsorbed systems
4. Conformational Analysis of molecules
5. Adsorption studies on mesoporous molecules
6. Classical Simulation module for pre-processing
7. Quantum chemistry simulator for homogenous (downstream conversions) and heterogenous (crackers) systems
8. Quantum Physics simulator for heterogenous systems (crackers)
9. Classical simulation for inorganic solids

Industry Solutions: Pharma and Biotech

Enabling API Development



Molecular Simulation

Vol. 34, Nos. 10–15, September–December 2008, 1353–1357



Empirical molecular modelling of suspension stabilisation with Polysorbate 80

Jamie T. Konkel^{a*} and Allan S. Myerson^{b1}

^aGlobal Research and Development, Baxter Healthcare, Round Lake, USA; ^bDepartment of Chemical and Biological Engineering, Illinois Institute of Technology, Chicago, USA

(Received 26 February 2008; final version received 24 September 2008)

Molecular modelling has been used successfully to predict the stabilisation of crystalline nanosuspensions of model pharmaceutical drugs by the surfactant Polysorbate 80. The ratio of the binding energy of the Polysorbate 80 to the binding energy of the drug to the surface of the crystal was found to correlate with the stabilisation of the nanosuspension.

Keywords: molecular modelling; Polysorbate 80; pharmaceutical; suspension

- **Background:** Formulation of poorly water-soluble drugs into crystalline nano-suspension.
- **Aim:** “Develop a molecular modelling approach to rapid surfactant screening, which could identify stabilising surfactant systems for a particular drug, based on its crystal structure.”

Industry Solutions: Pharma and Biotech

Applicable Material Studio Modules

1. MS Visualizer and Collection
2. MS Amorphous Cell
3. MS Adsorption Locator
4. MS Conformer
5. MS Sorption
6. MS Forcite (plus, COMPASS)
7. MS DMOL3
8. MS Reflex
9. MS Morphology
10. MS Polymorph

Functionality

1. 3D Sketch & Build, 3D volume, property and trajectory visualization
2. Preprocess, system construction, packing, etc.
3. Find minimum energy configuration for adsorbed systems
4. Conformational Analysis of molecules
5. Adsorption studies on mesoporous molecules
6. Classical Simulation module for pre-processing
7. Quantum chemistry simulator as property calculator and geometry optimizer for polymorph predictor
8. Powder pattern indexing and solving algorithms
9. Crystallite shape and sizes predictor
10. Polymorph predictor

Academia

Departments

Physics
NanoSciences
Electronics
Engineering
Materials

Chemistry
All the above
except CASTEP

Modules

MS Visualizer and Collection
MS Amorphous Cell
MS Adsorption Locator
MS Conformer
MS Sorption
MS Forcite (plus, COMPASS)
MS DMOL3
MS Reflex
MS Morphology
MS Polymorph

Applications

Band gap engineering
Electron Transport
Thermal and electrical conductivity
Core hole spectroscopy
Powder Solve with XRAY diffraction
Phonon, IR and RAMAN
Solid state NMR

Reaction kinetics and thermodynamics
UV-Vis spectra
IR and RAMAN

