CONCEPT

Computational Chemistry and Molecular Modelling: DFT, Force Fields and Catalyst Screening

31 May – 4 June 2027
London - Central London four-star



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Ref: 725_19219 **Date:** 31 May – 4 June 2027 **Location:** London - Central London four-star **Fees:** 23000 SAR

Introduction:

Industrial R&D groups in petrochemicals, catalysis and polymers spend months synthesising catalyst and additive candidates that a few well-chosen calculations could have ruled out, while other teams trust computed numbers that no experiment has checked. This Core Concept course equips chemists to apply computational chemistry and molecular modelling with judgement: force fields and molecular mechanics, density functional theory, geometry optimisation, transition states, molecular dynamics, spectroscopic and thermodynamic property prediction, QSPR surrogates and validation against measurement. Participants produce a Computational Screening Study Plan for a case catalyst or additive.

Course Objectives:

- Match an R&D question on a catalyst, additive or polymer to the lowest-cost computational method that can answer it to the accuracy the decision needs
- Build and check molecular mechanics models by choosing and testing a suitable force field family for organic, polymer or reactive systems
- Run density functional theory geometry optimisations, frequency checks and free energy corrections, choosing functional, basis set and dispersion treatment with stated reasons
- Locate transition states and compare reaction pathways and adsorption energies to rank catalyst candidates with descriptor and volcano plot reasoning
- Predict spectroscopic and thermodynamic properties and train QSPR or machine-learning surrogates with defined applicability domains
- Design a computational screening funnel with compute budget, workflow scripts and an experimental validation plan for a case catalyst or additive

Target Audience:

- Research chemists who design and evaluate catalyst, monomer and additive candidates in industrial laboratories
- Materials scientists responsible for polymer formulation, stabiliser and property development programmes
- Catalysis specialists who interpret activity and selectivity data and screen new active sites
- Process R&D staff who need thermochemical, kinetic and physical property data for new chemistries
- Analytical chemists who interpret IR, Raman and NMR spectra and want computed reference spectra
- Modelling and simulation staff who support laboratory teams with molecular calculations

Course Outline:

Day 1: Scope, Limits and Method Choice in Computational Chemistry

- Method Hierarchy: Molecular Mechanics, Semi-Empirical, Hartree-Fock, DFT and Correlated Ab Initio
- Accuracy Versus Cost Scaling and the Chemical Accuracy Benchmark
- Potential Energy Surface Concepts: Minima, Saddle Points and Conformer Searches
- Question Framing Canvas for Petrochemical, Catalysis and Polymer Modelling Requests
- R&D Portfolio Audit: Candidate Questions for Modelling Versus Bench Experiments

Day 2: Force Fields, Quantum Chemistry and Density Functional Theory

- Force Field Anatomy: Bonded Terms, Coulomb and Lennard-Jones Non-Bonded Terms
- Force Field Families: AMBER, CHARMM, OPLS, GAFF, TraPPE and Reactive ReaxFF
- Kohn-Sham DFT and the Exchange-Correlation Ladder: LDA, GGA, Meta-GGA and Hybrid Functionals
- Gaussian-Type Basis Sets Versus Plane Waves and Pseudopotentials for Surfaces and Solids
- Dispersion Corrections, Spin States and Known DFT Failure Modes

Day 3: Geometry Optimisation, Reaction Pathways and Molecular Dynamics Lab

- Geometry Optimisation Convergence Criteria and Vibrational Frequency Checks
- Reaction Energies, Zero-Point Correction and Gibbs Free Energy From Partition Functions
- Transition State Searches: Nudged Elastic Band and Intrinsic Reaction Coordinate
- Adsorption Energies and Descriptor-Based Catalyst Screening With Volcano Plots
- Molecular Dynamics Set-Up: Ensembles, Thermostats, Equilibration and Trajectory Analysis

Day 4: Property Prediction, QSPR Surrogates, Compute Workflows and Validation

- Spectroscopic Prediction: Computed IR, Raman and NMR Shifts With Scaling Factors
- Thermochemical Estimates: Heats of Formation, Implicit Solvation and Polymer Glass Transition From MD
- QSPR Descriptors and Machine-Learning Surrogates: Random Forest, Neural Networks and Y-Scrambling
- Batch Job Scripting, Workflow Managers and Calculation Data Provenance on Shared Compute
- Validation Against Experiment: Error Bars, Applicability Domain and Benchmark Sets

Day 5: Lab Capstone: Computational Screening Study Plan for a Case Catalyst or Additive

- Case Brief: Candidate Library for a Dehydrogenation Catalyst or Polymer Antioxidant Additive
- Method Selection Matrix and Compute Budget Estimate for the Screening Funnel
- Screening Funnel Design: Force Field Pre-Filter, DFT Ranking and Surrogate Model
- Experimental Validation Plan and Go or No-Go Criteria Linking Calculations to Bench Tests
- Computational Screening Study Plan Presentation and Peer Technical Challenge

Skills You Will Gain:

- Electronic Structure Method Selection
- Force Field Parameter Assessment
- Transition State Location
- Catalyst Descriptor Screening
- Molecular Dynamics Trajectory Analysis
- Computed Spectra Interpretation
- Surrogate Model Validation
- Simulation Workflow Provenance

Why Attend This Course:

- Leave with a Computational Screening Study Plan for a case catalyst or additive, challenged by peers from other R&D groups
- Cut the number of candidates sent to synthesis by ranking them first with calculations whose error you can state
- Question vendor and literature modelling claims by recognising unsuitable functionals, force fields and unvalidated surrogates
- Exchange modelling practice with chemists from petrochemical, catalyst, polymer and specialty chemical laboratories

Conclusion:

Calculations earn a place in industrial R&D when the method matches the question, the numbers carry stated error and the results are checked at the bench. The week moves from method hierarchy and potential energy surfaces through force fields and density functional theory, to geometry optimisation, transition states, molecular dynamics, property prediction, QSPR surrogates and compute workflows. The final day turns this into a Computational Screening Study Plan that links a candidate library to a validation programme.