

QM/MM for Biomolecules — Hands-on

Model chemistry in proteins with hybrid accuracy and scale. Learn to partition QM vs MM regions, choose embeddings, set up interfaces between QC engines and MD packages, locate transition states, and compute reaction free-energy profiles with transparent, reproducible outputs.

QM/MM for Biomolecules (Hybrid Quantum–Molecular Mechanics)

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Session 1

Fee: Rs 6300 [Apply Now](#)

Concepts: Partitioning & Embedding

Defining QM vs MM regions: chemistry coverage, size and boundaries

Theory

Capping strategies and boundary handling

link atoms (H) **pseudobonds** **frozen MM shells**

Embedding choices and charge treatment

mechanical/electrostatic embedding **polarizable**

embedding (overview) **charge derivation (RESP/ESP)**

Session 2

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Practical Setup: Engines & Interfaces

Connecting QC and MD codes; file plumbing & units sanity

ORCA/CP2K/Gaussian* **AMBER/CHARMM/GROMACS**
OpenMM **ChemShell/pmx (bridges)**

Level of theory selection for biomolecular QM regions

DFT (GGA/hybrid) **semiempirical (GFN/AM1/PM6)**
basis sets & dispersion

Equilibration and restraints around the active site

harmonic shells **positional restraints**

Session 3

Fee: Rs 11200 Apply Now

Reaction Paths, Sampling & Analysis

Locating TS and mapping mechanisms (overview)

constrained scans **NEB/string methods** **IRC (intrinsic reaction coord.)**

QM/MM-MD & free energy profiles along a coordinate

umbrella sampling **WHAM integration** **metadynamics**
(overview)

Uncertainty & robustness checks

window overlap **replicates/bootstraps** **sensitivity to**
QM region/level

Session 4

Fee: Rs 14000 Apply Now

Mini Capstone: Mechanism → ΔG Profile

Define QM region, map a key step, and assemble a ΔG profile (reaction coordinate)

Theory + Practical

Provenance & reproducibility checklist (inputs, levels, seeds)

protocol YAML **scene & figure exports** **tables & logs bundle**

Deliverables: figures, tables, README & manifest

PDF **CSV/TSV** **checksums**