HPRC Laboratory for Molecular Simulation (LMS)

https://lms.hprc.tamu.edu/

Subscription Rates for Texas A&M University Researchers FY23

Subscription Type	Number of Users with Access to LMS Software and Hardware	Consulting Hours Included	Cost per year
1	PI & 1 researcher	5	$500
2	PI & 2 researchers	10	$1000
3	PI & 3 researchers	15	$1500
4	PI & 4+ researchers	20	$2000
Consulting Fee for non-subscribers and additional hours for subscribers: $65/hour			

In addition to the consulting hours, an annual subscription to the LMS gives the PI and designated researcher(s) access to the licensed software and hardware outlined below.

Licensed Software	
Company	Software
Dassault Systèmes	**BIOVIA Materials Studio** Visualizer, Conformers, Forcite Plus, Gaussian Interface, QSAR+, Reflex, VAMP, MS Pipeline Pilot Collection, Adsorption Locator, Amorphous Cell, Blends, Compass, GULP, Mesocite, Mesodyn, Sorption, Synthia, CASTEP, DFTB+, DMOL3, NMR CASTEP, ONETEP, QMERA
Dassault Systèmes	**BIOVIA Discovery Studio** Visualizer, Analysis, Biopolymer, Catalyst (Conformation, Score DB Build, Search, Hypothesis, SBP & Shape), CHARMm, DMOL3, MMFF, Protein Refine, QUANTUMm, CFF FF, De Novo Evolution, De Novo Ligand Builder, Flexible Docking, LibDock, LigandFit, LigandScore, Ludi, MCSS, MODELER, Protein Docking: ZDOCK and RDOCK, Protein Families, Protein Health, Sequence Analysis, X-ray.
Materials Design	**MedeA Software** MedeA Environment (includes MedeA GUI, MedeA Analysis, MedeA Builders, MedeA JobServer and TaskServer, MedeA InfoMaticA, MedeA COD GUI, MedeA LAMMPS GUI, and MedeA Forcefield)
Schrödinger	**Schrödinger** suite of software: Maestro, CombiGlide, Glide, Liaison, Strike, QikProp, Canvas, LigPrep, BioLuminate GUI, Prime, Qsite, MacroModel, ConfGen, Jaguar, pKa Predictor, Epik, SiteMap, and PIPER.
CCG	**MOE**: Molecular Operating Environment. A fully integrated drug discovery software package, including structure-based design, fragment-based design, pharmacophore discovery, medicinal and biologics applications, protein and antibody modeling, molecular mechanics/dynamics, cheminformatics and QSAR.
Gaussian	**Gaussian** (09 & 16)
GaussView	**GaussView 6 with GMMX add-on**
Molpro	**Molpro**
SCM	**ADF & ADF-GUI**
TK Gristmill	**AIMALL Professional**
NBO	**NBO7**
Chemissian	**Chemissian**
Hardware:	
Computer	Configuration
LMS	10 Dell Precision T3420 workstations NVIDIA Quadro K620 GPU
MM	2060 core cluster. 76 20-core cpu nodes & 27 20-core gpu nodes (K20).