



**University School of Basic & Applied Sciences**  
**GGs Indraprastha University**  
Sector 16-C, Dwarka, New Delhi-110078

Date: 22/10/2018

**Notice Inviting Quotations**

Sealed quotations are invited from reputed companies/authorized dealers for supply of following softwares under the FRGS grant of PI- Dr. Kriti Batra, Assistant Professor, University School Basic and Applied Sciences, GGSIPU.

S.No.	Software	Quantity
1.	<b>Gaussian 16 64bit Multiprocessor Upgradation from 32bit Multiprocessor Single User Academic license on Windows</b>	1
2.	<b>GaussView06 Single User on Windows</b>	1

**Eligibility Criteria**

1. The Supplier should be a reputed and an authorized firm/supplier having after sales service agreement with the OEM (Proof for the same to be enclosed along with address, phone nos. & E-mail etc. of the Service Centre).
2. If ISO certified Company, enclose documentary proof.
3. The supplier should have experience of more than five years in execution and maintenance of software quoted (A certificate of establishment to be provided).
4. The quotations document complete in all respect should reach the Office of the PI-Dr.Kriti Batra, Room No.B-502, B Block, University School of Basic and Applied Sciences, GGS Indraprastha University, Delhi-110078 on or before 31/10/2018 by 2.00 pm. No quotations after the last date shall be entertained.

**Sequence of documents to be provided/ enclosed:**

1. GST certificate
2. PAN card document
3. Proof of the authorized agent/distributors/supplier.
4. Sole Proprietary/sole manufacturer certificate for proprietary item.
5. Document in support of list of similar software supplied by the firm to other Universities/Institutes with addresses and phone numbers of customers.
6. Name and address of registered office, Head Office and Regional office of the company with name and phone numbers of key persons.

*K. Batra*  
22/10/18  
DR. KRITI BATRA  
Assistant Professor  
University School of Basic & Applied Sciences  
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## Terms and Conditions

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18. In case replacement of a part becomes necessary during warranty period, the parts of the same make and same or better configurations as were originally there in the software shall be used. The supplier/vendor shall maintain details of the replacements and repairs carried out, if any, in a separate document and produce the details to the user department of GGSIPU. The cost of the parts will be borne by the supplier.

19. In case of complaint regarding repairing/replacement of software within the warranty period, the supplier will provide repair/replacement immediately. In case of noncompliance or delayed compliance, supplier will be penalized with an amount equal to 10% of the Bank Guarantee and would be deducted from the Bank Guarantee.

20. Delivery within 3-4 weeks otherwise the order will be considered as cancelled automatically and the EMD will be forfeited.

21. All corrigenda will only be notified on the GGSIPU website.

22. The Vice-Chancellor, GGSIPU shall be the final Authority for settlement of any dispute and his interpretation of any Clause/term/condition(s) of this document shall be final and binding and the jurisdiction for Court of Law shall be Delhi/New Delhi.

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Dr. J. S. Chahal  
Vice-Chancellor  
GGS Indraprastha University  
Sector-14, Connaught Place, New Delhi-110074

# Gaussian 16 Features at a Glance

## Fundamental Algorithms

Calculation of one- & two-electron integrals over any contracted gaussian functions, SCF solutions, automated fast multipole methods (FMM), pure DFT calculations, 1D, 2D, 3D periodic boundary conditions (PBC), Shared-memory (SMP), cluster/network and **GPU-based** parallel execution.

## Model Chemistries

**Molecular Mechanics, Ground State Semi-Empirical, Density Functional Theory** : EXCHANGE FUNCTIONALS, CORRELATION FUNCTIONALS, PURE FUNCTIONALS, HYBRID METHODS, DOUBLE HYBRID, EMPIRICAL DISPERSION, LONG RANGE-CORRECTED.

**Electron Correlation**: MP2 energies, gradients, and frequencies, MP3 and MP4(SDQ), Configuration Interaction (CISD), Coupled Cluster methods, Complete Basis Set (CBS) MP2 Extrapolation.

## Basis Sets and DFT Fitting Sets.

## Geometry Optimizations and Reaction Modeling

Geometry optimizations for equilibrium structures, transition structures, and higher saddle points, in redundant internal, internal (Z-matrix), Cartesian, or mixed internal and Cartesian coordinates, Newton-Raphson and Synchronous Transit-Guided Quasi-Newton (QST2/3) methods, of intrinsic reaction path following (IRC), applicable to ONIOM QM:MM, BOMD molecular dynamics (all analytic gradient methods); ADMP molecular dynamics: HF, DFT, ONIOM(MO:MM)

## Vibrational Frequency Analysis

normal modes (harmonic and **anharmonic**), Pre-resonance Raman spectra (HF and DFT), NMR shielding tensors & GIAO magnetic susceptibilities, Vibrational circular dichroism (VCD), Dynamic Raman Optical Activity (ROA), **IR intensities etc**

## Molecular Properties

: Mulliken, Hirshfeld, Natural Bond Orbital (NBO) analysis, Multipole moments, hyperpolarizabilities, optical rotary dispersion, Hyperfine spectra components, Electrostatic potential, electron density, density gradient, Laplacian, and magnetic shielding.

## ONIOM Calculations

Enhanced 2 and 3 layer ONIOM energies, gradients and frequencies, Support for IRC calculations, ONIOM integration of electric and magnetic properties.

## Excited States

Restartable time-dependent (TD) HF & DFT energies, gradients and **frequencies**, EOM-CCSD energies and **gradients**, **Franck-Condon**, **Herzberg-Teller** and **FCVT analyses**, CI-Singles and TD-DFT in solution, **electronic circular dichroism (ECD)**.

## Solvation Models

Polarized Continuum Model (PCM), SMD model, ., Isodensity Surface  
PCM (I-PCM) energies and Self-Consistent Isodensity Surface PCM (SCI-PCM) energies and gradients

## Integration with External Programs

NBO 6, COSMO/RS, **DFTB input file**, Keyword and **Link 0** command support

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# GaussView

## ***Build and Examine Molecules in 3 Dimensions***

Build structures by atom, functional group, ring, amino acid (central fragment, amino-terminated and carboxyl-terminated forms) or nucleoside, Open PDB files and other standard molecule file formats, including SDF and MOL2 multistructure files, Rotate even large molecules in 3 dimension, View molecules in several display modes, Build unit cells for 1, 2 and 3 dimensional periodic boundary conditions, Specify ONIOM layer assignments.

## ***Set Up Gaussian 16 Calculations***

Molecule specification input is set up automatically, Specify additional redundant internal coordinates by clicking on the appropriate atoms and optionally setting the value, Specify the input for any Gaussian 03 calculation type, Set up molecule specifications for QST2 and QST3 transition state, Start and monitor local Gaussian jobs, Easily stream log files from running jobs in a text-searchable window.

## ***Visualize Gaussian16 Results***

Show calculation results summary, Examine atomic changes, Create surfaces and contours for molecular orbitals, electron density, electrostatic potential, spin density, or NMR shielding density from Gaussian job results, Animate normal modes associated with vibrational frequencies, Display spectra: IR, Raman, NMR, VCD, ROA, UV-Visible, Animate geometry optimizations, IRC reaction path following, Display 3D surface plots for 2-variable scan calculations, Produce web graphics and publication quality graphics files and printouts.

## ***Extra Features:***

PCM Solvation Cavity, Anharmonic Frequency Analysis, Vibronic Spectra, Enhanced Calculation Summary, Saving Movies, Symmetry, One Step Multi-Job Setup

*J. Baker*  
22/10/18