



গড়গাঁও মহাবিদ্যালয়  
GARGAON COLLEGE

**Department of Chemistry**  
**Add on /Certificate program**

No of hours: 30 hours

Subject: Computational Chemistry

Number of students enrolled: Twenty students

**Banner:**

**Computational Chemistry**  
To provide foundation of theories, techniques and softwares for computational chemistry  
**AIM & outcome**  
Incultation of computational chemistry literacy. ability to understand & critically evaluate quality and applicability of computational chemistry methods and results in scientific literature

**Intake Capacity: 15**  
**Course Fee: Rs 400/-**  
**Duration: 1 month**  
<https://drive.google.com/file/d/13fafADKNa4QAeVtEFeoZ8pzHm7D8bctj/view?usp=sharing>

**INSTRUCTORS**  
Dr. A. Narzary  
Dr. P. Begum  
Ms. S. S. Begum

**GARGAON COLLEGE**  
contact coordinator  
Saheen Shehnaz Begum  
7002560074  
<https://forms.gle/e7xL4H5popsF31Xz5>  
computationalchemgc@gmail.com

**ADD-ON COURSE**  
course Approved by  
*Dibrugarh University*  
<https://forms.gle/e7xL4H5popsF31Xz5>

## **Add-On Course**

### **Computational Chemistry**

This course is designed for students having a basic understanding of quantum chemistry and use of computers in general. This is a 30-hour course divided into 5 units with the target of attaining the following course outcomes.

Course outcomes:

CO1: Computer Literacy in Chemistry: A central goal of this course is to make the student a “computer literate” chemist having a good understanding of the uses of computers in chemistry. The computational techniques are currently used to predict the structure and properties of molecules. The focus of the course is to familiarize with the existence, uses and limitations of various computational tools.

CO2: Understanding and application of Molecular mechanics calculation to simple system

CO3: Understanding and application Quantum mechanical calculation to simple systems

CO4: Introduction of students to Molecular Dynamics simulation techniques and its varied applications in chemistry.

Course Content:

Unit 1 [3 lectures]

Introduction to computational chemistry: utilisation and limitations of computational chemistry, basic theories and tools of computational chemistry

Unit 2: [5 lectures]

Use of computational tools for drawing molecular structures in chemistry: ChemDraw, Avogadro, Isis draw, UCSF Chimera, ChemSketch, MarvinSketch, ChemCraft.

Unit 3: [5 lectures]

Quantum Chemistry: Basics of Hartree-Fock method, basis sets, basics of density functional theory, DFT based reactivity descriptors. Introduction to popular softwares: Gaussian, DMol, Discovery Studio. Applications to simple molecular systems.

Unit 4: [5 lectures]

Methods in Computational Chemistry: Molecular Mechanics, Docking Techniques and Molecular Dynamics. Basic principle and geometrical description of small molecules,

intermolecular interactions, origin and modelling of dispersion forces & hydrogen bonds; Integration of the Newton's equations: initial conditions.

Unit 5:

[12 lectures]

Hands on experience: Using Gaussian for verification of bond length, bond angle, structure optimisation, energy calculations for small molecules- CO, NO, CO<sub>2</sub>, H<sub>2</sub>O, NH<sub>3</sub>, HCl, HBr, HF, HI, other similar moieties; Using AutoDock for docking ligands/ligand-like molecules onto macromolecules such as proteins and scan for most compatible ligand for that system; MD Simulation of ligand in macromolecular system and further analysis via xmGrace.

After completing the course, students shall be able to:

- draw the molecular structures of chemical compounds that are used as the starting point of any calculation in computational chemistry
- explain the most important principles for quantum chemical and molecular mechanic methods of computing the geometry and energy of molecules
- plan and apply computer-based calculations to determine the geometry, energies and electronic properties of molecules.
- describe theoretical methods and plan and conduct computer-based calculations of chemical properties
- critically examine and discuss the results from computer-based results for chemical moieties.

Text Book(s)

1. Lewars, E. Computational Chemistry, (Springer, 2003).
2. Cramer, C. J. Essentials of Computational Chemistry (Wiley 2002).
3. Balagurusamy, E. Numerical Methods, (Tata McGraw-Hill Publishing Company Limited, 2002).

Reference Book(s)

1. Leach, A. R. Molecular Modeling: Principles and Applications, 2nd Edn., (Pearson Prentice Hall, 2001).
2. Jensen, F. Introduction to Computational Chemistry (Wiley 1999).

**List of students are:**

Sl. No.	Name of the Student	Semester
1.	Bikramaditya Phukan	5 <sup>th</sup>
2.	Ashish Gogoi	5 <sup>th</sup>
3.	Mrinal Phukon	5 <sup>th</sup>
4.	Ankita Chetia	5 <sup>th</sup>
5.	Stuti Buragohain	5 <sup>th</sup>
6.	Sandhanee Phukon	5 <sup>th</sup>
7.	Abhishruti Gogoi	5 <sup>th</sup>
8.	Pritom Phukon	5 <sup>th</sup>
9.	Roshmi Devi	Graduated
10.	Nikita Debgupta	Graduated
11.	Bishwajeet Changmai	5 <sup>th</sup>
12.	Suman Chetia	3 <sup>rd</sup>
13.	Himadree Gogoi	3 <sup>rd</sup>
14.	Bobita Arandhara	3 <sup>rd</sup>
15.	Dimpi Borah	3 <sup>rd</sup>
16.	Chimpi Boruah	3 <sup>rd</sup>
17.	Lakhipriya Baruah	3 <sup>rd</sup>
18.	Niharika Deka	3 <sup>rd</sup>
19.	Rekha Borah	3 <sup>rd</sup>
20.	Hapi Moni Gogoi	3 <sup>rd</sup>

Browser tabs: Inbox (3,774) - saheenshehnaz@, Classes, Add On Course

URL: classroom.google.com/u/1/c/NTMSNTgyMTlwMDUw

### Add On Course

Stream Classwork People Grades

Class code: **bbzxix**

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**Saheen S Begum** Sep 3, 2022

For today's class try this:  
Based on the lecture and demonstration yesterday, all of you can go ahead and try downloading GaussView in your computers via the link:  
<https://webintopc.com/gaussview-6-0-16-free-download/>  
(Password 123)  
Also go through: the pdf attached here.  
Leave your attendance in the comments here before 4 pm.

**intro2gaussview.pdf**  
PDF

4 class comments

**Ashish Gogoi** Sep 3, 2022  
Ashish Gogoi  
5th sem  
142

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URL: meet.google.com/qfg-akch-bkt?pli=1&authuser=0

### Meet - qfg-akch-bkt

8:28 PM | qfg-akch-bkt

Nikita debgupta	Roshmi Devi	Mrinal Phukon	Suman Chetia	Rekha Borah
Stuti Buragohain	Bishwajeet Changmai	Lakhipriya Boruah	Ankita Chetia	BIKRAMADITYA PHUKON
chimpi Boruah	Dimpi Borah	Bobita Arandhara	Niharika Deka	Abhishruti Gogoi
Himadree Gogoi	Sandhaneer Phukon	Ashish Gogoi	Hapimoni Gogoi	You

People

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In call

- Saheen Shehnaz (You) Meeting host
- Abhishruti Gogoi
- Ankita Chetia
- Ashish Gogoi
- BIKRAMADITYA PHUKON
- Bishwajeet Changmai
- Bobita Arandhara
- chimpi Boruah

System tray: Windows, Taskbar, System tray (Network, Volume, Power), Date: 20:28 13-06-2022