

# **A SHORT TERM COURSE ON: COMPUTATIONAL CHEMISTRY**

**Organised by:**

**DEPARTMENT OF CHEMISTRY  
HINDU COLLEGE**

**In collaboration with:**

**DEPARTMENT OF PHYSICS  
STOCKHOLM UNIVERSITY, SWEDEN**

**PHYSICS GROUP  
BHABHA ATOMIC RESEARCH CENTER  
MUMBAI**

**DEPARTMENT OF CHEMISTRY  
J.V. COLLEGE, BARAUT, U.P.**

## **SPEAKERS AND CONTENT DEVELOPERS**



**Dr. Michael Odelius**

**Professor  
Department of Physics  
Stockholm University,  
Sweden**



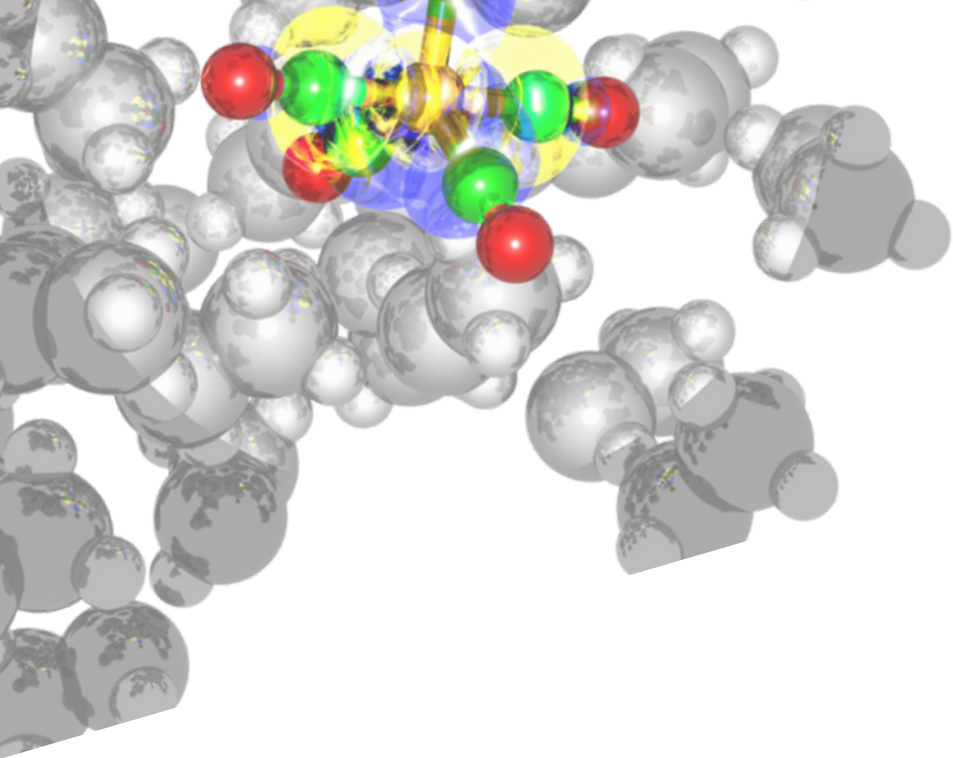
**Dr. Shyam Kishor**

**Associate Professor & Head  
Department of Chemistry  
J.V. College Baraut, U.P.**



**Dr. Lavanya M. Ramanaiah**

**Scientist  
Physics Group  
Bhabha Atomic Research  
Centre, Mumbai**



## Concept Note

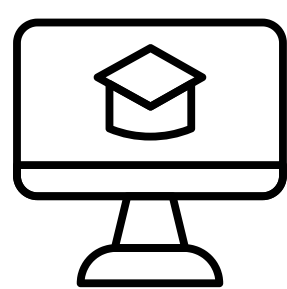
**Computing** has altered our reality. It has simplified the way that we live and the way that we practice science. The entire research enterprise has received huge impetus over the past two decades as scientists and engineers have put the advances occurring in computing to direct use. This revolution is based on the utilization of massively parallel high performance computers to solve the complex equations that describe natural phenomena, e.g., the Schrödinger equation for electronic motion in molecules or Newton's equations of motion for the classical motion of hundreds of thousands of particles such as those in a protein. Computational Chemistry has influenced our understanding of the way the world works, it has helped the manufacturers design more productive and efficient processes, characterized new compounds and materials, and helped other researchers extract useful knowledge from mountains of data. It essentially has provided qualitative/quantitative insights into experimental work and has guided the choice of which experimental system to study or enable the design of new systems.





## About Hindu College

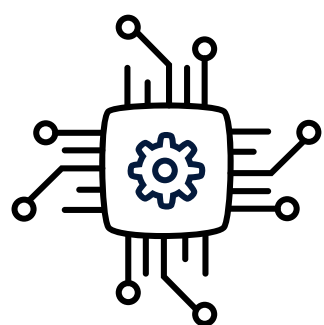
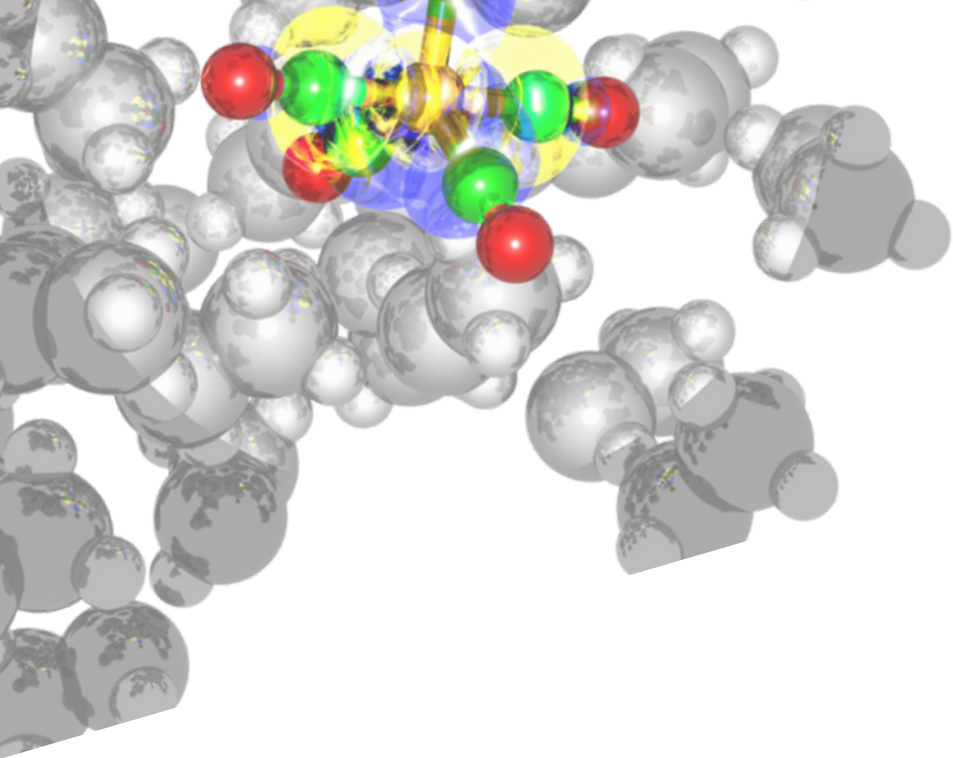
Hindu college is one of the most distinguished and prestigious co-educational institutions of our country with a recognized history of 121 years. After receiving A+ grade in NAAC accreditation, the college has been placed first in India Today Rankings 2020 and is also consistently being placed among the top three colleges of our country by NIRF. The college offers 39 undergraduate and postgraduate courses in Science, Humanities and Social Sciences. The Department of Chemistry, Hindu College has been one of the most acclaimed and well known Departments across the country. The college endeavors to nurture students with a keen analytical and scientific bent of mind with a sensitivity to their responsibilities. To promote research and innovation, the college is coming up with a dedicated art research centre.



## About Stockholm University

Stockholm University is a public university in Stockholm, Sweden, founded as a college in 1878, with university status since 1960. Stockholm University has over 65 departments and fifteen research institutes and centres, and offers 75 master's programmes and three bachelor's programmes taught in English within two scientific areas, human sciences and science, with four faculties – humanities, law, social sciences and natural sciences, making it one of the largest universities in Scandinavia. The university has a strong international research profile with particular focus on fundamental research and is regarded as one of the top 100 universities in the world by the Academic Ranking of World Universities (ARWU).

Four Nobel Laureates in Chemistry, and the appointment of the world's first female professor of Mathematics in 1889, mark the university's proud history. Stockholm University College was founded as a bold project, a modern university in the spirit of Enlightenment, with the aim of serving society and continues to build on this foundation as an open, innovative, and dynamic university.



# About the Course

Participants of this course will learn how to use open source molecular editors & visualizers for:

Building molecules small and large (organic as well as inorganic)

Building materials (crystal structures, polymers, CNTs, quantum dots, etc.)

In this, an introduction to quantum chemistry is included with detailed insight into Hartree-Fock (HF) theory, introducing fundamental concepts of the molecular orbital theory along with the limitations of the HF method. The Kohn-Sham formulation of density functional theory is briefly presented and related to HF and post-HF calculations. Coupled with practical exercises, the lectures give a basic understanding and familiarity with quantum chemical methods for solving the molecular Schrödinger equation.

During the course, using open-source Quantum Chemistry codes, the following questions will be answered:

How to find and verify equilibrium and transition state geometries?

How to perform a detailed study of the

(a) Ground state structures and energetics?

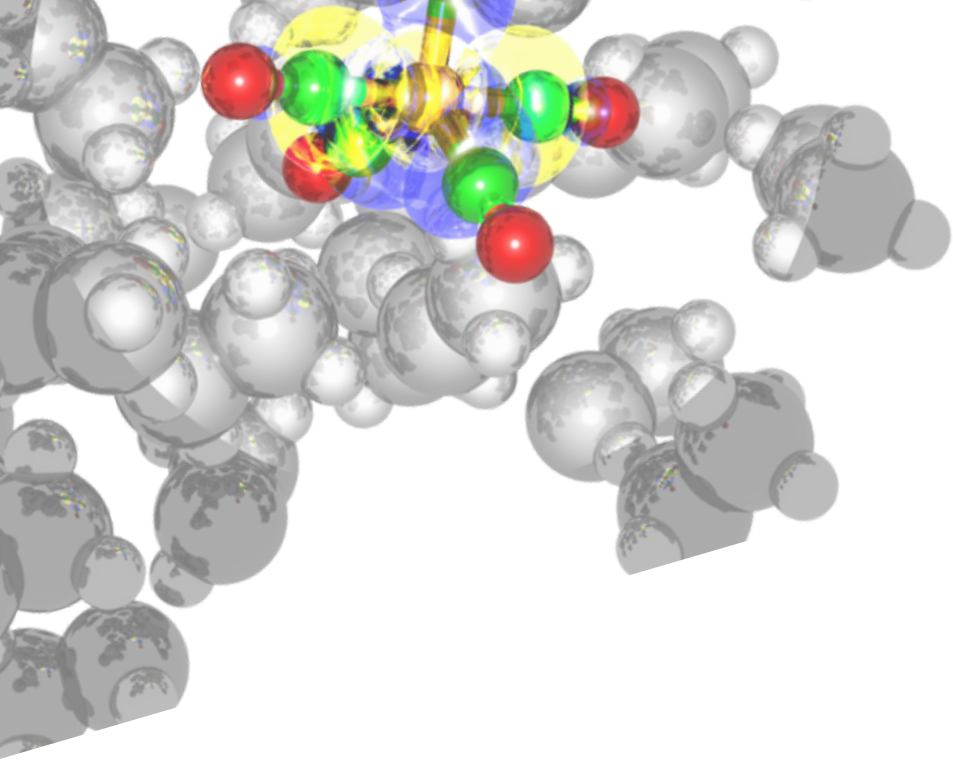
(b) Chemical properties such as ionization potential, electron affinity and reactivity descriptors such as electronegativity chemical potential, chemical hardness/softness etc.?

(c) Thermodynamic properties (Heats of Formation etc.)?

How to describe chemical reactivity using frontier molecular orbitals?

How to use Computational Chemistry techniques to efficiently calculate UV/VIS spectra, IR spectra, Raman spectra and NMR spectra?





## Programme Details

The course will commence in the first week of February.

**It will be a self-paced course with recorded lectures being provided weekly.**

The evaluation will be done on the basis of these lectures and the corresponding assignments.

 Course Duration: 3 MONTHS

Fee: Rs. 500/-

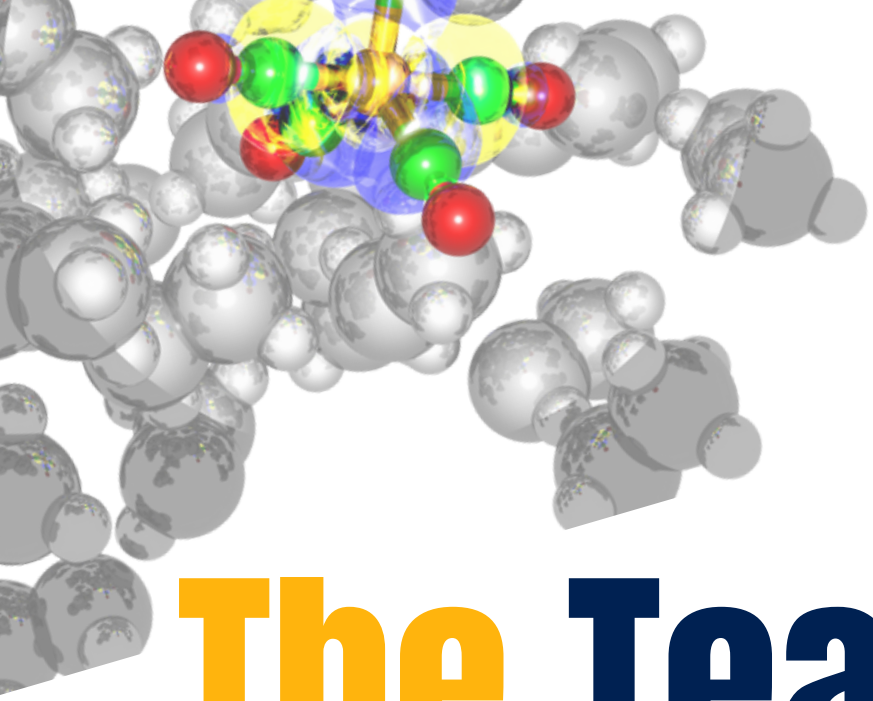
## How to Apply?

The process of Application will be a two-step procedure.

YOU HAVE TO REGISTER FIRST VIA THE FOLLOWING  
REGISTRATION LINK: [HTTPS://FORMS.GLE/R4MCIPOXVAKRWRO8](https://forms.gle/R4MCIPOXVAKRWRO8)

The link to the payment will be sent to you via email or via WhatsApp.

There are only a limited number of seats that shall be filled on a "First come First Serve" basis.



# The Team

## Content Developers

Dr. Michael Odelius: Professor, Department of Physics, Stockholm University, Sweden

Dr. Lavanya Ramanaiah: Scientist, Physics Group, Bhabha Atomic Research Centre, Mumbai

Dr. Shyam Kishor: Associate Professor & Head, Department of Chemistry, Janta Vedic College, Baraut, U.P.

## Advisors

Dr. Anju Srivastava, Principal, Hindu College.

Dr. Reena Jain, Vice Principal, Hindu College

## Coordinators

Dr. Geetika Bhalla, Department of Chemistry, Hindu College

Dr. Devanshi Magoo, Department of Chemistry, Hindu College

Teacher Assistant : Kalpana Jain, Research Scholar

### **Student Coordinators:**

Ms. Arsha Choudhary, Ms. Ashu Neha Hemrom, Mr. Dhruv Aggarwal,  
Ms. Sneha Chourasia, Ms. Sumedha Sengupta, and Ms. Yashna Dawar

### **For any Queries, Contact:**

Ms. Arsha Choudhary: 9068723271, choudharyarsha92@gmail.com

Mr. Dhruv Aggarwal: 9354367813, dhrugagg1712@gmail.com

Ms. Sumedha Sengupta: 9650122452, sumedha.s148@gmail.com