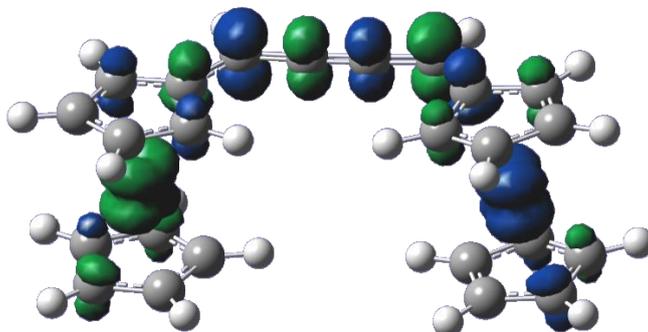


Manipal Centre for Natural Sciences
Centre of Excellence
Short certificate course on

Chemistry with Computer



Dr. Suranjan Shil

Assistant Professor, Chemistry group

Course duration: May 23-27, 2022

Format: Interactive classes on 23rd, 25th and 27th May 2021, from 5:30 pm to 7:00 pm together with additional reading /activities, on 24th and 26th May.

Venue: Microsoft Teams online platform.

About the course: In present-day research of chemical science largely depends on computation because of the accurate and fast prediction of chemical properties. In this course, I will try to give a brief idea about what we can do in chemistry using computers and the underlying theoretical background. The course will deal with hands-on experience in chemical property calculation like thermochemistry, molecular orbital, spin states, magnetic property, reaction mechanism, etc.

Topics to be covered: Basics of Hartree-Fock theory, basics of Density Functional Theory (DFT), basis sets, calculation of thermochemical properties, the energy of spin states, spin density, molecular orbitals, transition state, electron density, magnetic exchange coupling constant, magnetic anisotropy, etc.

Who can apply: Students enrolled in M.Sc. chemistry or physics with basic knowledge of quantum chemistry. Lifelong learners who wish to get an overview of the field are also welcome.

How to apply: The number of participants is limited to 30. Use the following link for the application

https://forms.office.com/Pages/ResponsePage.aspx?id=Qr2-Kf_xPUyWiAZ-NGDcH3VGzcQ57hdHk68LkF5NEr9UNIJKQzFLTjY1NDU5N0ZJTDVFN0NOSjIzTi4u

Selected candidates will be notified through email. **There is no registration fee.**

Eligibility for the completion certificate: 100% attendance and completion of all the modules in the course.

Contact details: MCNS office: Phone no: +91 820 2923571

Email: office.mcns@manipal.edu