About the Conference

Computational chemistry has become an essential approach in nearly every area of molecular science, including catalysis, biophysics, environmental science, and spectroscopy. It has emerged as an essential tool, just like common laboratory techniques such as nuclear magnetic resonance (NMR) spectroscopy, infrared (IR) spectroscopy, and mass spectrometry (MS). Calculations can provide significant insight at the atomic-level into mechanisms, dynamics, and processes, and can provide accurate predictions of molecular properties. The development of new methods and algorithms, combined with technological advances are driving the field forward, providing pathways towards addressing new chemical challenges, enabling computational approaches to be used increasingly more proactively, such as towards the design of new molecules and reactions.

The complexity of the challenges that computational chemistry methodologies are able to address is growing rapidly. Simulations are becoming increasingly accurate, while being able to access experimentally relevant timescales for large systems. Electronic structure methods are being used in new areas. Yet, there are many new, exciting challenges that computational chemists need to address such as potential of computational techniques based on the principles of quantum mechanics to extract structural information pertaining to quantum crystallography, interactions in strongly correlated systems, and addressing chemistry at the interface are important areas that are, in many ways, remain as some of the holy grails of computational chemistry, needing further developments.

The aim of this conference is to spark discussion and ideas towards the future of computational chemistry. The talks will focus on method development and state-of-the-art applications across computational molecular science, and will include discussion about newer and forthcoming technologies. The schedule of outstanding speakers covers a wide range of computational disciplines. We will encourage cross-fertilization between areas.

About the Departments

SAIF, Panjab University was created by Department of Science and Technology, Govt. of India. during the 6th Five-Year Plan. The complete facilities of SAIF/CIL are working in unison to provide analytical services and practical training to researchers and scientists throughout the country. It houses TEM, SEM, FESEM, NMR (400 MHz), PXRD, WDXRF, LC-MS, GC-MS, CHN-SO analyzer, FTIR UV-Vis-NIR Spectrometers.

Call for Papers

The participants are requested to submit the abstract(s) (maximum 250 words) of their paper(s) typed in MS word, Times New Roman font, 12 point with single spacing on A4 size with 3 cm right and 5 cm left, 1.5cm top and bottom margins through email to Dr. Neetu Goel (Convener)at compchemconference@gmail.com as an attachment in MS word format with above said specifications. The name of the presenting author of the poster should be underlined. Poster size should be 1m x 1m in dimension. The participants interested in making oral presentation should send an email to the above mentioned email address.

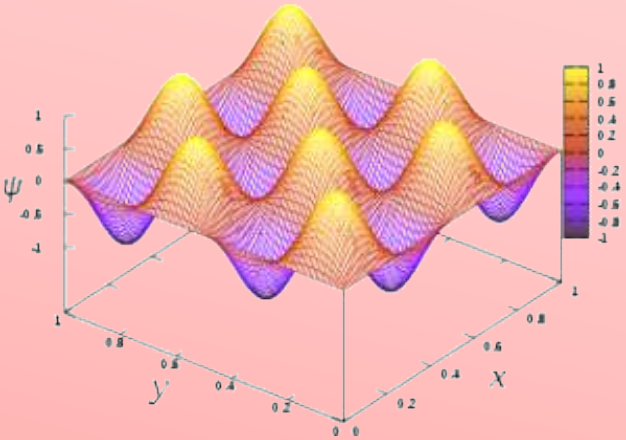
Conference

on

STRATEGIES AND CHALLENGES IN COMPUTATIONAL CHEMISTRY

from Molecular Simulation to Quantum Crystallography

March 5-6, 2019



Venue
Department of SAIF/CIL
Panjab University, Chandigarh

Sponsored by:
DST PURSE-II

Organizing Committee

Prof. S. K. Mehta – Chair
Prof. K.N. Singh
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Dr. Shuchi Gupta
Er. H. P. S. Kang
Er. Poonam Kumari
Dr. Ramesh Sharma
Er. Anil Kumar Sharma

Confirmed speakers

Prof. G. N. Sastry
(Chief Scientist G, IICT-Hyderabad)

Prof P. V. Bharatam
(Professor of Medicinal Chemistry at NIPER, S.A.S. Nagar, Mohali)

Prof. Michael Springborg
(University of Saarland, Saarbrucken, Germany)

Dr. Girinath G. Pillai
(Chief Scientific Officer Zastra Innovations, Bengaluru)

Dr. Abir De Sarkar
(Scientist-E & Dean (Academics), INST, Mohali)

Dr. M. Molayem
(University of Saarland, Saarbrucken, Germany)

Dr. C. S. Bera
(Scientist C, INST, Mohali)

Accommodation

The participants may be provided accommodation at the university guest houses/hostels based on the availability. Please send requests for accommodation in advance.

About Chandigarh

Chandigarh is one of the most beautiful and well planned cities in India, designed by the French architect Le Corbusier. Serenity and a city are normally two diametrically opposite concepts, which however, get belied in the 'City Beautiful'. Chandigarh is a rare epitome of modernization co-existing with nature's preservation. The city is located near the foothills of the great mountains of Himalayas with the Queen of Hills, Shimla.

About Panjab University

Panjab University is one of the oldest Universities in India established in 1882. University campus is spread over an area of 550 acres in sectors 14 and 25 of the city of Chandigarh. It ranked 1st among the Universities in India and 38th in Asia, in Times Higher Education Asian University rankings 2015. Panjab University has a long tradition of pursuing excellence in teaching and research in science and technology, humanities, social sciences, performing arts and sports. PU campus attracts and supports the best minds and recruits faculty who excel at teaching and research. University has 75 teaching and research departments and 15 Centers

Registration

Early Bird Registration-Before 28/02/2019

Academia 1000 INR (students)
Academia 2000 INR (faculty/scientists)
Industry 4000 INR

Late Registration-After 28/02/2019

Academia 1500 INR (students)
Academia 2500 INR (faculty/scientists)
Industry 4500 INR

The registration fee can be deposited in cash or sent by Demand draft drawn in favour of **Director, SAIF, Panjab University**, payable at Chandigarh.

Contact Us

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