

The first DAE-CCS symposium is being organized by Chemical Engineering Group, Bhabha Atomic Research Centre (BARC), Trombay, Mumbai, India, during November 7-9, 2019. The symposium is supported by the Board of Research in Nuclear Sciences (BRNS), Department of Atomic Energy (DAE). The field of computational chemistry is growing rapidly with the continuing development of computer power, new and robust algorithms, and the availability of scalable software. Computer simulations provide a direct route to generate macroscopic properties of molecular systems of experimental interest through microscopic information. Today, computational chemistry can provide useful estimates of the properties and behavior of materials even before they have been synthesized and evaluated through experiments. The purpose of the symposium is to create a platform for scientists and engineers, especially for the young researchers for an effective interaction amongst of those engaged in research in the area of computational chemistry, as it will be attended by eminent scientists and engineers from national laboratories, universities and research institutes across India.

Scope of the symposium

- A. Fundamental studies on structures, thermodynamics and transport properties
- B. Metal ion and Isotope separation
- C. Water purification
- D. Reaction mechanism and catalysis
- E. Nanomaterials and polymers
- F. Hydrogen and other gas storage materials
- G. Chemical biology
- H. Radiation damage in materials

The scientific programme of the symposium will include invited talks by eminent scientists from India. The invited talks will encompass basic studies and applications and will address various advanced topics which include novel solvent design, high capacity nanoadsorbents, robust membranes for desalination and fuel cells, identification of composition of glass for vitrification, high capacity hydrogen storage materials, mechanistic pathway of enzyme catalyzed reactions, interaction of radiation with matter and many more. Contributed papers will be presented in poster sessions. Further, the best poster presentations will be selected for the awards. Abstract of the contributed papers will be peer reviewed prior to their inclusion in the symposium's proceedings. Limited number of selected papers will be considered for publication in journals of international reputation. The prior intimation will be given to authors about the selection of their contributions for consideration of journal publication.

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ABSTRACT SUBMISSION

Contributory papers are invited on topics listed in the scope in the form of two pages manuscript in specified format. The entire text should be typed in MS Word, paper size A4 (210 x 297 mm), page margins: top 25 mm, bottom 25 mm, left 25 mm and right 25 mm. The font should be Times New Roman (font 12) with single line spacing. Manuscript should be categorized (A to H) as per the titles given under SCOPE of the symposium.

The manuscript should be submitted by e-mail to daeccs2019@gmail.com; daeccs2019@barc.gov.in

E-mail ID of corresponding author should be given in the manuscript and presenting author should be underlined. All the future communications in respect of manuscript will only be made to corresponding author. DAE participants may please note that the contributed papers should be accompanied with scanned copy of the note of approval from the competent authority. There will be award for best posters.

Registration fee

Research student/Postdocs	Rs. 1000/-
Faculty/Scientist	Rs. 4000/-
Participants from industry	Rs. 8000/-

Registration fees will be accepted only through crossed cheque/crossed DD/Net banking system to the following account

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