

CFCAM Sponsored Event

Advances and Challenges in Biomolecular Simulations: The Biennial Meeting of the International Society for Quantum Biology and Pharmacology 2021

<https://isqbp2021.sciencesconf.org>

Tuesday June 29, 2021 to Thursday July 1, 2021

Organizers

Dr. Roland H. STOTE

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Introduction and motivation

The International Society of Quantum Biology and Pharmacology (ISQBP) is a non-profit society founded in 1970 to provide a forum for chemists, pharmacologists and biologists to discuss and extend the impact of computational methodologies in the fields of biology, chemistry, chemical biology, medicinal chemistry, pharmacology, bioinformatics, genomics and proteomics. To achieve the mission of the ISQBP, the outgoing president, relying essentially on registration fees and sponsorship, organizes a biennial meeting for scientists working in the areas of molecular modelling, theoretical chemistry, computational biology and informatics as a means to nurture interactions with those performing experimental studies as well as with other disciplines to foster interdisciplinary research. The organizer of the 2021 meeting is Dr. Roland H. Stote, the current president of the ISQBP, in conjunction with the Institute of Genetics, Molecular and Cellular Biology (IGBMC), one of the main biomedical research centers in Europe. The 2021 Congress will celebrate the 51st anniversary of the creation of the ISQBP.

State of the art

Previous meetings of the ISQBP have gathered up to ca. 120 scientists from all over the world and have taken place in Ascona, Switzerland (2008), Cetraro, Italy (2010), Stockholm, Sweden (2012), Telluride, U.S.A. (2014), Bergen, Norway (2016) and Barcelona, Spain (2018). This edition, in 2021, will take place **on line given the current sanitary pandemic**. As it has been for the previous meetings, the program of the 2021 meeting will feature about 15 keynote invited speakers and an equal number of presentations by young scientists, selected on submitted abstracts. These will include PhD students and postdocs in order to offer a platform for young researchers to present and discuss their work with their peers. The size of the meeting (ca 120 participants) will allow for ample discussions between all participants. **The online conference, besides talks, will include poster sessions.**

The program includes plenary lectures by world-renowned speakers and high quality papers to be selected from the abstracts submitted.

The program includes plenary lectures by invited speakers and papers selected from the abstracts submitted, poster sessions, as well as pauses to facilitate discussion between participants and speakers. The talks generally cover a variety of topics reflecting the latest advances in the field of biomolecular simulations applied to macromolecules of biological interest, in particular, proteins and nucleic acids. The conferences and poster presentations involve leading foreign researchers coming from institutes in the United States, Spain, Sweden, Portugal, Norway, as well as French researchers. The ISQBP 2021 congress represents a unique opportunity to present local and national expertise, establish contacts and promote interactions between international academic and industrial researchers. The reputation of the ISQBP is attested to by the many leading scientists who have been associated to or have received awards from the organization; many are pioneers in the field and the list includes Nobel Prize winners. The 2021 Congress will celebrate the 51st anniversary of the creation of the ISQBP.

Objectives

The objective of the meeting is to facilitate interactions between chemists, pharmacists and biologists in the field of molecular modelling and *in silico* biology.

Given the difficult times we have experienced in the past 18 months due to the COVID pandemic; many in the scientific community lament the loss of international interactions. This congress will bring together about 120 participants from around the world to present and discuss topics covering a vast field of research at the chemistry-biology interface (rational design of molecules of therapeutic interest, molecular recognition, dynamics of biological macromolecules, enzymatic catalysis) and are of interest to scientists from both academic research and the industrial world, in particular the pharmaceutical industry. Current participants number largely from Europe, but also North and Central America, as well as Asia. The congress is aimed at senior researchers, thesis students and young post-doctoral researchers in fields focused on biomolecular computing, molecular modeling and simulations, and biochemoinformatics. For the young researchers, the congress is an opportunity to inform themselves beyond their current research projects, to meet renowned scientists and make useful contacts for their future professional integration.

Participant List

Invited/Confirmed Speakers

Charles L. Brooks, III, University of Michigan, USA, brookscl@umich.edu
Marco Cechinni, University of Strasbourg, France, mcecchini@unistra.fr
Thomas E. Cheatham, University of Utah, USA, tec3@utah.edu
Carmen Domene, University of Bath, UK, mcdn20@bath.ac.uk
Franca Fraternali, Kings College, London, UK, franca.fraternali@kcl.ac.uk
William Jorgensen, Yale University, USA, william.jorgensen@yale.edu
Klaus Liedl, Leopold-Franzens-University Innsbruck, Austria, Klaus.Liedl@uibk.ac.at
Alex MacKerell, University of Baltimore, USA, alex@outerbanks.umaryland.edu
Adrian Mulholland, University of Bristol, UK, adrian.mulholland@bristol.ac.uk
Lennart Nilsson, Karolinska Institutet, Sweden, lennart.nilsson@ki.se
Modesto Orozco, University of Barcelona, Spain, modesto.orozco@irbbarcelona.org
Montgomery Pettitt, University of Texas, USA, mpettitt@utmb.edu
Carol Post, Purdue University, USA, cbp@purdue.edu
Maria Ramos, University of Porto, Portugal, mjramos@fc.up.pt

Plus ~10 speakers chosen from the collection of submitted abstracts, currently under review.

Plus ~95 other participants, including poster presenters and simple participants.

Financial Support

Preliminary Budget

Congress title: Advances and Challenges in Biomolecular Simulations: The 2021 ISQBP

President's Meeting (Virtual)

Date: 29 June – 1^{er} July 2021

Organizing research unit: IGBMC UMR 7104

Project organizer : Roland H. Stote

| Expenses | Amounts (€) Excluding tax (HT) | Receipts | Amounts (€) Excluding tax (HT) | |
|--|---|--|-----------------------------------|-------------|
| | | | Received | Requested |
| Communication | | Subventions | | |
| Publicity | 1500 | Université de Strasbourg | 2500 | 2500 |
| | | ACS journal JCTC | 450 | 450 |
| Other | | | | |
| Video conference organization by PremC | 8500 | ISQBP | 700 | 700 |
| | | <u>CECAM-FR-MOSER</u> | | <u>2500</u> |
| Logistic organization IGBMC | 1000 | Inscriptions (as of 26/05/2021) | | |
| | | Student early-bird: (31.82HT, 35 TTC) | | 955 |
| | | Participant early-bird: (63.64HT, 70 TTC) | | 3167 |
| | | Student regular: (40.50HT, 45 TTC) | | 364 |
| | | Participant regular: (72.73HT, 80 TTC) | | 364 |
| TOTAL expenses | 11000 | TOTAL receipts | | 11000 |