INFORMATION

#### CIC IN SHORT

"Chemistry-Information-Computer (CIC)" is a division of the German Chemical Society (Gesellschaft Deutscher Chemiker e.V.) covering the research area where computational methods are applied for rational molecular design, virtual screening, materials simulations, prediction of biological and physical properties from chemical structure, organisation and visualisation of chemical data. Founded in 1982, CIC brings together scientists from various disciplines to foster and propel development and applications in this field, with particular emphasis on

- the annual German Conference on Chemoinformatics (CIC workshop),
- promotion of chemoinformatics, computational chemistry and chemical information as part of the curriculum at universities and higher teaching institutions,
- support of working groups on particular aspects of interest to CIC.
- organising courses on CIC working methods and techniques.
- promoting cooperation and knowledge exchange between universities and industry.
- supporting the open source idea for the development of chemistry software in the academic environment,
- stering the relationship between international institutions working in this field in particular to EuCheMS and ACS,
- usage of modern communication platforms like blogs and social networks.

http://www.gdch.de/cic http://twitter.com/GDCh CIC

#### SPONSOR

All sponsors may be found on the www.gdch.de/gcc2016 website.

If you are interested in sponsoring or exhibiting please contact gcc@dr-kirsten.de for more information.

#### ACCOMMODATION

Fulda is located at the heart of Germany and famous for its baroque old town. The conference hotel "MARITIM Hotel am Schlossgarten" is within 10 minutes walking distance from Fulda main station. The hotel provides accommodation for participants in single or double bed rooms

Alternatively low-priced accommodations are available in the IBIS Hotel or in the Holiday Inn Fulda.

For more information see our conference webpage:

#### www.gdch.de/gcc2016

Arrangements should be made directly with each hotel under the keyword "GCC 2016" not later than September 4, 2016.

The customers will be held accountable for non-occupancy of reserved rooms.

#### **▶** INFORMATION ABOUT THE SCIENTIFIC PROGRAMME

Dr. Thomas Engel LMU München Faculty of Chemistry and Pharmacy Butenandtstr. 5-13 81377 Munich, Germany

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# **▶ INFORMATION ABOUT THE ORGANISATION**

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Phone: +49 69 7917-358 E-mail: tg@gdch.de

Homepage: www.gdch.de/tagungen

Executive Director: Professor Dr. Wolfram Koch

Registered Charity No: VR 4453 · Registergericht Frankfurt am Main

Date: 01.03.2016/TG



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GESELLSCHAFT DEUTSCHER CHEMIKER



Fachgruppe
Chemie – Information – Computer

GCC 2016

12<sup>th</sup> German
Conference on Chemoinformatics

November 6 – 8, 2016 FULDA · Germany

www.gdch.de/gcc2016



The division Chemistry-Information-Computer (CIC) of the German Chemical Society (Gesellschaft Deutscher Chemiker e.V.) cordially invites you to participate in the

## 12th German Conference on Chemoinformatics November 6 – 8, 2016, FULDA

## VENUE

MARITIM Hotel am Schlossgarten Fulda Pauluspromenade 2, 36037 Fulda, Germany

## ▶ AIM OF THE CONFERENCE

The conference will reflect and highlight the new role of cheminformatics in the modern information world. It will span a wide range of subjects related to the use of computers in chemistry, pharmacy, materials science and biology; from chem- and bioinformatics to explicit modelling and from industrial applications to fundamental academic research. The scientific programme will include plenary and contributed lectures, posters and software presentations. The language of the conference is English.

#### CONFIRMED INVITED SPEAKERS

Andrea Cavalli Bologna/IT Jonas Bostrom Mölndal/SE Friedrich Foerster Utrecht/NI Francesco Gervasio London/UK Val Gillet Sheffield/UK Francesc Illas Barcelona/ES Josef Scheiber Munich/DE Anne Wassermann Boston/US **Tony Williams** Durham/US

current speaker list at:

#### www.gdch.de/gcc2016

# SOFTWARE WORKSHOPS

The conference programme contains a slot for several software workshops. Our sponsors will introduce the participants into the latest software developments in our research area.

If you are interested in providing or contributing to this slot please contact either Dr. G. Kirsten or Dr. Oliver Koch (see below) for more information.

# **EXHIBITION AND SPONSORS**

Companies interested in providing workshops, exhibit or sponsor the conference, please contact Dr. G. Kirsten at gcc@dr-kirsten.de for more information.

#### ▶ SCIENTIFIC COMMITTEE

Frank Böckler Tübingen/DE Tim Clark Erlangen/DE

Thomas Engel Munich/DE (CIC Division and Conference Chair)

Jon Essex Southampton/UK
Uli Fechner Frankfurt/DE

Guido Kirsten Cologne/DE (Conference Co-Chair)

Oliver Koch Dortmund/DE Jan Kriegl Biberach/DE Frank Oellien Ludwigshafen/DE Matthias Rarey Hamburg/DE Gisbert Schneider Zurich/CH Josef Scheiber Munich/DE Halle/DE Wolfgang Sippl Alexander Tropsha Chapel Hill/USA Wendy Warr Holmes Chapel/UK Gerhard Wolber Berlin/DE

## **TOPICS**

Big Data

Chemical Information

Chemoinformatics and Drug Discovery

Databases

Data handling

In silico Tox Prediction

\* Material Sciences

\* Molecular Modelling

Protein Modelling

Quantum chemical calculations

Simulations

Structure Determination

Solvation

# **▶** ORAL COMMUNICATIONS AND POSTERS

For scientific contributors we offer three different formats: Talk (20 min.), Research telegram (12 min.) and poster. Research telegrams are reserved for Ph.D. students to give the opportunity to present the highlights of their research to a wider audience.

Please submit an abstract of your contribution exclusively via internet at:

## www.gdch.de/gcc2016

Sample abstracts can be found on this website. No editing is done by the scientific committee. You will receive a reference code for each submission.

The scientific committee reserves the right to accept, reject papers or assign them to a different format.

#### SCHOLARSHIPS

Scholarships will be offered to a limited number of students, candidates for doctor's, diploma's, bachelor's or master's degree presenting a scientific contribution (main author of an oral contribution or poster). Please send your application to GDCh until **August 30**, **2016** latest.

Please follow the corresponding link at our conference webpage:

#### www.gdch.de/gcc2016

#### POSTER AND LECTURE AWARD

Prizes will be awarded for the two best posters and the best talk of junior scientists within the "Research Telegrams".

#### CIC AWARD FOR COMPUTATIONAL CHEMISTRY

We invite research group leaders to propose excellent German candidates for the CIC award for Computational Chemistry for excellent master and doctoral theses within the period of summer 2015 – summer 2016.

Details are published on the CIC webpage:

## www.gdch.de/cic

## REGISTRATION

Please register online not later than **September 30, 2016** (early bird registration until **July 15, 2016**) by using our online form at:

#### www.gdch.de/gcc2016

For detailed registration fees see our conference webpage.

#### DEADLINES

Submission of oral contributions May 31, 2016
Submission of Research Telegrams May 31, 2016
Submission of posters August 30, 2016
Scholarships August 30, 2016
Room Reservation September 4, 2016
Registration deadline September 30, 2016

(No guarantee for last-minute-posters to be published in the book of abstracts)