REGISTRATION

REGISTRATION

Please register online at
http://processnet.org/en/JTR_FrankfurtI_2017.html.
In general there is no registration deadline as long as free capacity is available. Confirmation of registration and the invoice will be sent after receipt of the registration. Conference tickets and list of participants will be available at the registration desk on site.

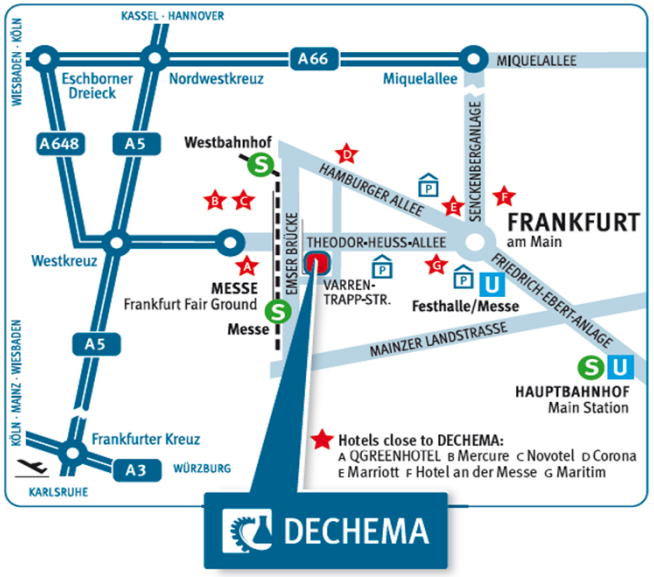
GENERAL INFORMATION

VENUE / ORGANISER

DECHEMA e.V.
Theodor-Heuss-Allee 25
60486 Frankfurt/Main
Germany

CONTACT

Dr. Rolf Lenke
Phone: +49 (0)69 7564-267
Fax: +49 (0)69 7564-304
E-Mail: lenke@dechema.de

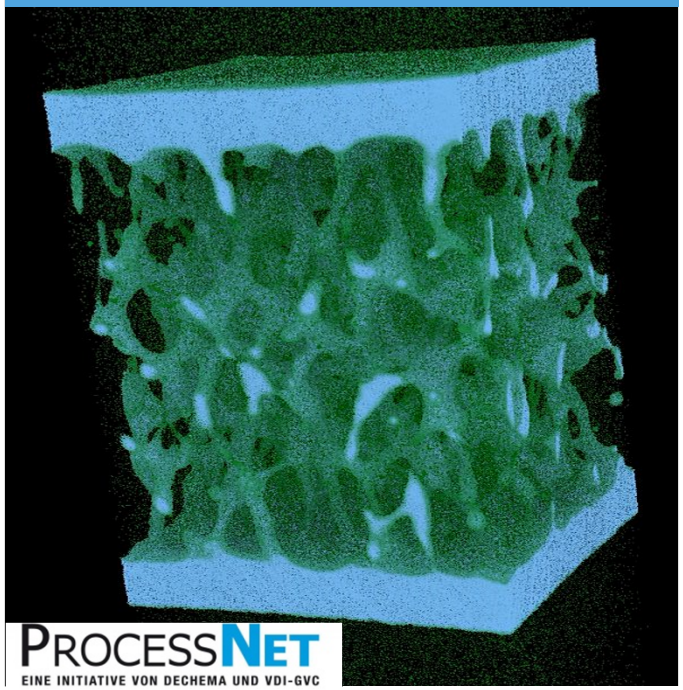


DECHEMA VDI

CALL FOR PAPERS

9./10. March 2017
DECHEMA-House - Frankfurt/Main - Germany

International Workshop
Molecular Modeling and Simulation: Science, Engineering and Industrial Applications



INVITATION / PROGRAMME COMMITTEE

Molecular modeling and simulation are of key methods in research in many areas of physics, chemistry and biology, but also in engineering. Simulation methods and tools are now available in this field, which enable addressing not only scientific but also practical problems. They yield new insights and contribute to finding novel solutions in industrial research and development.

The international MolMod workshops are dedicated to this rapidly developing interdisciplinary field in which science and engineering join forces. They provide a unique opportunity for getting an overview of the state of research in molecular modeling and simulation at the interface between science and engineering. Moreover, they bring together experts from academia and industry, as well as from different scientific communities that are engaged in applied molecular modeling and simulation.

MolMod 2017 will be held in downtown Frankfurt/Main, Germany, one of Europe's most easily accessible cities, and will start on Thursday morning 9. March 2017 at 11 a.m. and close on Friday afternoon 10. March before 5 p.m. A social program is organized for Thursday night.

PROGRAMME COMMITTEE

H. Hasse TU Kaiserslautern
C. Holm University of Stuttgart
J . Vrabec University of Paderborn
R. Lenke DECHEMA e.V.

The workshop is supported by:
ProcessNet Working Party on Molecular Modeling and Simulation for Process and Product Design
(Chairs: H. Hasse, Kaiserslautern/DE, J . Vrabec, Paderborn/DE)

DFG-Sonderforschungsbereich (SFB) 716 "Dynamische Simulation von Systemen mit großen Teilchenzahlen"
(Speaker: C. Holm)

SPEAKERS / TOPICS

CONFIRMED INVITED SPEAKERS

Daniel Borgis Ecole Normale Supérieure de Paris/FR
Walter G. Chapman Rice University/US
Ioannis Economou Texas A&M University at Qatar/QA
Jürgen Horbach Heinrich-Heine-Universität Düsseldorf/DE
Marcus Müller Georg-August Universität Göttingen/DE
Roland Netz Freie Universität Berlin/DE

TOPICS

Contributions should be related to applications of Molecular Modeling and Simulation that are of potential interest for solving practical problems in industry. The scope also includes the development of methods and experimental work related to or combined with molecular modeling and simulation. Major areas of interest are:

- Quantum Chemical Methods
- Force Fields
- MD/MC Simulation Methods and Tools
- Multiscale Modeling and Simulation
- Physico-Chemical Properties
- Polymers
- Reactive Systems
- Nanoscale Processes
- Porous Media
- Processes at Surfaces

SUBMISSION OF ABSTRACTS

Authors wishing to present a paper are asked to submit a single page abstract by **16. November 2016** via file upload on the internet at

dechema.de/JTR_FrankfurtI_2017_Beitragseinreichung.html

Please note that this is a very strict deadline and papers cannot be accepted after that date! You will find a template for preparing your abstract on the website.

The selection of the presentations, orals and posters, will be based on the review of the single page abstracts (max. size 500 kb, incl. figures) by the Scientific Committee. The abstracts should explicitly mention objectives, new results, and conclusions or significance of the work. The congress language will be English.

Please note that authors have to pay the full registration fee.