GERMAN BUNSEN SOCIETY FOR PHYSICAL CHEMISTRY– ANNUAL SCIENTIFIC CONFERENCE

SCIENTIFIC ORGANISATION

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Jürgen Gauß	University of Mainz
Manfred Kappes	Karlsruhe Institute of Technology
Willem M. Klopper	Karlsruhe Institute of Technology

LOCAL ORGANISATION

Artur Böttcher	Karlsruhe Institute of Technology
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ATTENTION!
Deadline for submission of abstracts is December 15, 2012

KARRIEREFORUM

The "Karriereforum" (career forum) is an annual symposium organised by the Karriereforum working group of the DBG. It aims at scientists in earlier stages of their careers (between PhD and first appointment as a professor), and provides a forum for discussion of and exchange on career related issues and questions. The annual symposium features 3-5 invited talks and an open discussion on a central career planning-related topic.

STUDENTS TRAVEL GRANTS

The foundation of the Bunsen Society provides financial support for the participation of students **(Ph.D. students are not eligible)** at the conference. Universities are requested to submit a joint list of eligible students on behalf of their research groups no later than **January, 31st 2013** to the Bunsen Society. The lists should contain information on the status of the students, their scientific qualification and economic situation. Furthermore, the lists should rank students according to the priority to receive travel grants.

PUBLICATION OF A THEMED PCCP ISSUE

"Theory meets Spectroscopy"

PCCP will publish the official themed issue to be displayed at the Bunsentagung entitled "Theory meets Spectroscopy" and guest edited by Manfred M. Kappes and Willem M. Klopper (both at Karlsruhe Institute of Technologdy). These two guest editors would be responsible for experiment (Kappes) and theory (Klopper).

Deadline for Submission:
November 30, 2012

All authors are invited to submit regular articles of original, unpublished research with a focus on quantum chemical methodology for spectroscopy or on the interplay between theory and experiment in spectroscopic studies in the gas or condensed phase, to PCCP.

All submissions will be subject to rigorous peer review against PCCP's high standard in the regular way. The guidelines for authors and the submission procedure can be found at: **www.rsc.org/pccp**.

High-quality submissions of original work in other areas of physical chemistry, chemical physics and biophysical chemistry are of course always welcome for publication in regular issues of PCCP.

EXHIBITION & SPONSORING

Companies are invited to participate at the accompanying exhibition. The exhibition presents a perfect opportunity to inform participants of your products and services and network with the participants. There are also various sponsoring opportunities available.

If you are interested in either exhibiting or sponsoring, please contact the local organisers directly (bunsen2013@ipc.kit.edu).

MEETINGS OF THE BUNSEN SOCIETY

THURSDAY, MAY 9, 2013

09:00	Board Meeting of the Bunsen Society (Vorstandssitzung)
09:00	Meeting of the education committee (Unterrichtskommission)
09:00	Meeting of the topics committee (Themenkommission)
11:00	Meeting of the Standing Committee of the Bunsen Society (Ständiger Ausschuss)
	Participants of the above meetings will receive separate invitations.
15:00	General Assembly of the Bunsen Society for Physical Chemistry (members only)

PROGRAMME OVERVIEW BUNSENTAGUNG 2013

THURSDAY, MAY 9, 2013

11:30	"Karriereforum"
16:30	Formal Opening of the Bunsentagung
19:30	Welcome Reception

FRIDAY, MAY 10, 2013

Scientific Programme and Poster Session

SATURDAY, MAY 11, 2013

Scientific Programme, Closing Ceremony and Conference Dinner

REGISTRATION FEES[1)]

Personal Members of the Bunsen Society	110.– €
Non-Members	140.– €
Students[2)] (proof of status required, no Ph.D. students))	35.– €
Invited Participants	0.– €
Accompanying Persons	25.– €

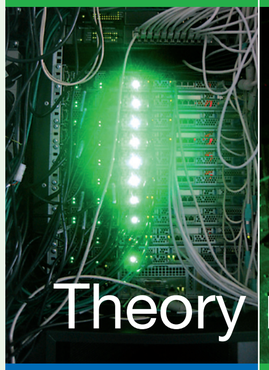
1) No VAT requested according § 4.22 USTG
2) Students enrolled in Bachelor and Master Courses only. Ph.D. students will be charged the regular registration fee.

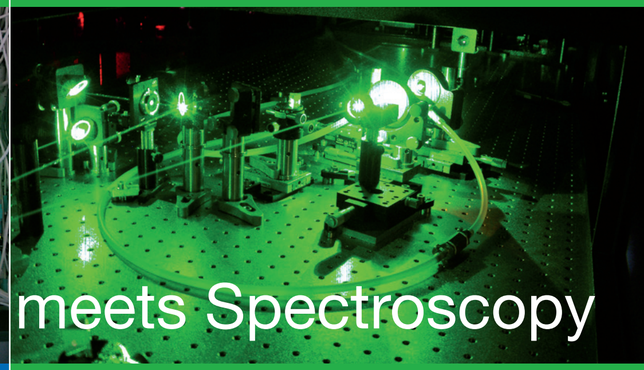
Late registrations after March 27, 2013 are subject to an additional registration fee of 20.– €/person (except accompanying person fee).

www.bunsentagung.de

First Announcement and Call for Papers

May 09 – 11, 2013 · Karlsruhe · Germany





Theory meets Spectroscopy

BUNSENTAGUNG 2013

112th General Assembly of the German Bunsen Society for Physical Chemistry

Also featuring a special symposium „Electrochemical Interfaces", an industrial symposium with accompanying exhibition, and the „Karriereforum"

www.bunsentagung.de

„Theory meets Spectroscopy“

Main Topic: Theory meets Spectroscopy
Special Symposium: Electrochemical Interfaces
Industrial Symposium: Physical Chemistry in Industry and Industrial Exhibition

The main topic of the Bunsentagung 2013 focuses on state-of-the-art research in the fields of theoretical spectroscopy as well as molecular characterisation using experimental spectroscopy guided by quantum chemistry. This also includes recent advances in experimental techniques that probe molecules in gas and condensed phases under precisely defined/controlled conditions as well as new developments in describing such systems theoretically at a predictive level.

There is a long-standing research synergy between molecular spectroscopy and quantum chemistry. Both fields are interested in eigenstates and how these can be interconverted by electromagnetic radiation. In the last ten years, new experiments have increasingly been stimulated by computational predictions while theoretical approaches have often benefited from experimental benchmarks. This trend will accelerate further due to recent developments in both theory and spectroscopic measurement. Experimental advances include methods which allow for better-defined samples (e.g., mass and conformer selection of large molecular ions, ultralow temperature cooling schemes, surface immobilization methods, etc.) and their spectroscopic characterisation at highest frequency and time resolutions. This has in turn enabled spectroscopic probes and spectroscopic control of chemical change at unprecedented levels of precision – with ramifications for fields ranging from nanoscience and catalysis to photo- and biophysical chemistry. In the last decades, novel quantum-chemical methods have been developed at a breathtaking pace, and as such they continue to be developed further. Today, a large variety of spectra can be simulated, many spectroscopic properties can be computed, larger molecular systems can be treated than before (e.g., in the framework of density-functional theory), and an extreme accuracy can be achieved (e.g., using coupled-cluster theory for rotational spectroscopy). Advanced time-dependent methods have been developed as well as efficient computational models to describe surface-bound systems and molecules in condensed phases (e.g., QM/MM methods, embedding schemes, and molecular dynamics simulations). Much recent work has been concerned with predictive-level treatments of electronically excited states and (non-radiative) transitions.

The main topic of the 112th Bunsentagung seeks to highlight the growing importance of the synergetic interplay between theory and spectroscopy in advancing the field of molecular chemical physics in the age of Moore´s law. As rapidly increasing computational resources become available, some areas of experiment are already being supplanted by predictive-level theoretical spectroscopy. Other areas of experimental spectroscopy, concerned with more complex molecular systems, can presently help to further develop theory by providing benchmarks. Finally, certain areas of molecular spectroscopy (e.g., under extreme conditions) will remain inaccessible to accurate computational prediction for quite a while yet. Nevertheless, even here useful physical insight will result from quantum-chemical model calculations.

The talks of this symposium are intended to illustrate and further encourage this synergy between modern spectroscopy and state-of-the-art quantum-chemical calculations – in terms of examples ranging from molecules in gas-phase, through surface-bound to interacting-in-condensed-phase.

LECTURES

OPENING LECTURE — Thursday, May 09, 2013

Comparing molecular photofragmentation dynamics in the gas and liquid phases
Prof. Dr. Mike Ashfold (University of Bristol/UK)

PLENARY LECTURES — Friday, May 10 and Saturday, May 11, 2013

Multidimensional spectroscopy of photophysics and photochemistry
Prof. Dr. Tobias Brixner (University of Würzburg/D)

Theoretical spectroscopy from molecular dynamics
Prof. Dr. Dominik Marx (Ruhr-Universität Bochum/D)

Insights into transition metal catalysis from a combination of spectroscopy and quantum chemistry
Prof. Dr. Frank Neese (Max Planck Institute for Bioinorganic Chemistry, Mülheim/D)

Interfacial charge transfer dynamics and femtochemistry of molecular adsorbates
Prof. Dr. Martin Wolf (Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin/D)

FULL LECTURES — Friday, May 10 and Saturday, May 11, 2013

Ultrafast soft X-ray photoelectron spectroscopy at liquid water microjets
Prof. Dr. Bernd Abel (University of Leipzig/D)

Evolution of Kondo resonance from a single impurity molecule to the two-dimensional lattice**
Prof. Dr. Maki Kawai (University of Tokyo/J)

Modeling environment effects on spectroscopies through QM/classical models
Prof. Dr. Benedetta Mennucci (University of Pisa/I)

Rotational spectroscopy meets theory
Prof. Dr. Cristina Puzzarini (University of Bologna/I)

IR and UV spectra of cold, biomolecular ions – a challenge for theory
Prof. Dr. Thomas Rizzo (Ecole Polytechnique Fédérale de Lausanne/CH)

Twenty years of battle with the NO_3 molecule: some things that I have learned
Prof. Dr. John Stanton (University of Texas at Austin, TX/USA)

** Tentative title

PROGRAMME COMMITTEE

Wolfgang Domcke	TU München, Garching
Marcus Elstner	Karlsruhe Institute of Technology
Karin Fink	Karlsruhe Institute of Technology
Jürgen Gauß	University of Mainz
Manfred Kappes	Karlsruhe Institute of Technology
Matthias Kling	Max Planck Institute of Quantum Optics, Garching
Willem M. Klopper	Karlsruhe Institute of Technology
Matthias Olzmann	Karlsruhe Institute of Technology
Marcell Peuckert	Infraserv GmbH & Co. Höchst KG, Frankfurt am Main
Martin Quack	ETH Zürich/CH
Dominik Samuelis	Max Planck Institute for Solid State Research, Stuttgart
Rolf Schäfer	TU Darmstadt
Rolf Schuster	Karlsruhe Institute of Technology
Dusan Velic	International Laser Centre, Bratislava/SK
Manfred Wilhelm	Karlsruhe Institute of Technology
Christof Wöll	Karlsruhe Institute of Technology
Rudolf Zentel	University of Mainz

SUBMISSION OF ABSTRACTS

We invite you to submit your contributions either to the main topic area or to any other topical areas. Submissions of contributions covering fundamental or applied, experimental or theoretical work (and combinations) are equally highly appreciated.

Topical areas

1) **Theory meets Spectroscopy (main topic)**
2) **Biophysical Chemistry**
3) **Solid State**
4) **Liquid State**
5) **Gaseous State**
6) **Interfaces**
7) **Soft Matter**
8) **Physical-Chemical Methods (experimental or theoretical)**
9) **Electrochemical Interfaces (special symposium)**

Submissions for the main topic should be in English. Submissions to the other topics can be made in English or German. **The authors are expected to present their work in the language of the abstract submitted.**

Abstract submission is accessible via
www.bunsentagung.de
from November 1, 2012 onwards.

Deadline for abstract submission: **December 15, 2012**
Abstracts submitted after this deadline will not be reviewed.

Authors are requested to submit an abstract (max. 1 page, 100-200 words) electronically as rich text format (.rtf) or Word format (.doc or .docx) via the abstract submission tool at **www.bunsentagung.de**. A template will be available at the website.

The abstracts of all accepted contributions will be published in a book of abstracts.

The Scientific Committee will review the submitted abstracts. Abstracts will either be accepted for oral or poster presentation. Abstracts might be rejected if their content is not within the scope of the conference or lacking scientific quality. The Scientific Committee might relocate contributions to other topical areas, if considered to be more relevant. Authors will be informed in February 2013 about the acceptance of their papers.

Requirements for successful submission of abstracts:
- Abstract to be submitted in the proper format
- Name and contact details of presenting author
- Name and institutional details of all authors
- Title of contribution
- Preferred topical area and preferred format of presentation (oral or poster)

Please follow the guidelines below when writing your abstract:
- Title: Arial 14 pt, bold
- Author(s): Arial 12 pt (first name and surname), presenting author underlined
- Institution / Location: Arial 12 pt
- Main Text: Arial 12 pt, line separation: 1,5 times
- Literature: Arial 12 pt
- Page Format: A4, at least 2,5 cm margin on all sides
- File Size: Max 300 kB

No header or footer, no page numbers

The scientific programme will be available at **www.bunsentagung.de** in April 2013.

ATTENTION!
Deadline for submission of abstracts is December 15, 2012