

Announcements

International Discussion Meeting of the Deutsche Bunsengesellschaft
für Physikalische Chemie

Molecular Spectroscopy and Molecular Dynamics – Theory and Experiment

Grainau, Oberbayern, Hotel am Badersee
28 August to 1 September 1994

an International Conference sponsored by The Deutsche Forschungsgemeinschaft
organized by W. Kutzelnigg, Lehrstuhl für Theoretische Chemie, Universität
Bochum, M. Quack, Laboratorium für Physikalische Chemie, ETH Zürich

The conference aims at bringing together theoreticians and experimentalists interested in the dynamics of molecules as derived from molecular spectroscopy in order to discuss problems of particular current interest. Exciting new developments in experiments on high resolution molecular spectra and their analysis as well as new theoretical developments in the calculation of such spectra and the related time independent and time dependent quantum dynamics of molecules have lead to new answers but also new questions in the field of intramolecular kinetics, molecular reaction dynamics, molecular chaos, and statistical mechanics. The current status of the field will be assessed with particular stress on fundamental aspects and new directions will be sought for. The meeting allows for invited lectures, contributed lectures and poster sessions. All sessions will be plenary.

Interested participants should contact: Prof. Dr. Martin Quack, Laboratorium für
Physikalische Chemie, ETH Zürich Zentrum, CH-8092 Zürich, Switzerland

Electronic Structure Methods for Truly Large Systems: Moving the Frontiers in Quantum Chemistry

Braunlage (Harz), Germany
August 1–7, 1994

Sponsored by: Deutsche Forschungsgemeinschaft
Ministerium für Wissenschaft und Kultur des Landes Niedersachsen

Directors: K. Jug (Germany), M. C. Zerner (USA)

Advisory Committee: G. Pacchioni (Italy), N. Rösch (Germany), R.D. Salahub (Canada)

The major goal of the workshop is to get together leading experts in quantum chemistry on ab initio, density functional, semiempirical and hybrid methods to report and discuss recent progress in methodology and application suitable for very large systems. Participation will be limited to about 60 invited participants. The program will include invited lectures (35 minutes plus 10 minutes discussion), invited posters and a panel discussion on the future of quantum chemistry. The program will cover the following areas: basic formalism, organic and inorganic compounds, biomolecules, clusters, solids.

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