

# The Darmstadt workshop on molecular modeling: Past and future

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*The majority of the contributions in this issue of the Journal of Molecular Graphics are papers that were presented at the Seventh Darmstadt Molecular Modeling Workshop, which took place at the Technical University Darmstadt on May 18–19, 1993. The technical organization of this workshop was again in the hands of the physical chemistry staff of the Technical University, Darmstadt, as it has been for the past six years. The scientific program was coordinated by Stefan Kast from the author's research group. The Darmstadt Workshop has been quite an informal and inexpensive event throughout the years. From 1994 onward, it will also be a specific meeting of the recently founded German-speaking branch of the Molecular Graphics Society. The following notes should help to provide an overview of the past activities and present some ideas for the future of this meeting.*

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## HISTORY

The first workshop was organized on June 4–5, 1987, by the author and his colleagues. It was the result of an initiative by the German Ministry of Science and Technology and is a forum for those German scientists who have been supported by the Ministry within the biotechnological program "Alternative Methods to Experiments with Animals."<sup>1</sup> The central aim of this first workshop was to bring scientists from universities and central state research institutions together with investigators from chemical and pharmaceutical companies in order to present the results of common activities in the field of computer-assisted drug design and to establish new cooperations. Sixty scientists participated and approximately 30 of them were from chemical industries.

During the final discussion of this first meeting, the participants voted for a continuation of the workshop in Darmstadt in the following years and voted that the local organization should remain in the hands of the author's research group, but the responsibility for the program should alternate between scientists from chemical and pharmaceutical companies to universities and state research centers. It was also decided to keep the "private" character of the workshop (i.e., to abstain from inviting several keynote

speakers and therefore minimize the organization's expenses and give, in particular, emerging scientists the chance to present their most recent results). This idea is still in use today.

The second workshop was organized in 1988 by Dr. H. Bruns, Merck cooperation Darmstadt, and his colleagues. The organizers focused the workshop topic on the calculation of molecular properties, but other fields were also presented. The workshop took place the two days before Ascension Day on May 10–11 and nearly 90 participants took part. Since the second meeting, it has become a tradition to hold the workshop on the two days before Ascension Day in May. The reason for this choice is obvious. The annual meeting of the Deutsche Bunsengesellschaft für Physikalische Chemie traditionally starts on Ascension Day and the organizers wanted to combine the two events so that both could be attended in only one journey.

The third workshop on May 2–3, 1989, was organized by Dr. D. Schomburg from the Gesellschaft für Biotechnologische Forschung (a state research center in Braunschweig) and his colleagues. The focus of the papers presented was on computer-aided protein design. The character of the workshop became even more clear during this third workshop. It was, in the majority, the young scientists who presented their most recent work and not the established group leaders.

The program of the fourth workshop in 1990 (May 22–23) was organized again by the author and his colleagues. The central topics were force fields and nonbiological polymers. At this workshop, the number of participants exceeded 100 for the first time. The main reason for this increase was definitely related to the fact that, for the first time, participants from the former East Germany were able to come to Darmstadt.

In the fifth year (May 7–8, 1991), the scientific program of the workshop was organized by Dr. H.-J. Boehm and his colleagues from BASF in Ludwigshafen. They focused the program on molecular recognition and chemical reactions. Close to 150 participants came to this meeting—a number that has remained almost constant to this date.

In 1992 (May 26–27), the scientific program was organized by Dr. C.-W. van der Lieth from the German Cancer Research Center (DKFZ) at Heidelberg. He focused the program on the interrelation between spectroscopy and molecular modeling. For the first time, commercial companies in the hardware and software industry presented their products in a demonstration session.

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The form of the organization of the 1992 workshop was continued in the 1993 meeting (including the software and hardware demonstration session). The program focused on molecular recognition and on new methods in molecular dynamics (MD) and Monte Carlo (MC) simulations. For the first time in the workshop's tradition, this event was supported by the Molecular Graphics Society (MGS), which paid travel expenses for the young scientists, who gave excellent presentations. Some of the contributions to the seventh workshop are published in this issue of the *Journal of Molecular Graphics*.

## FUTURE

In December 1993, the German-speaking branch of the Molecular Graphics Society was founded in Darmstadt by Dr. Tim Clark from the University of Erlangen, Dr. Hans-Peter Weber from SANDOZ in Basel (the organizer of the 1993 annual meeting of the MGS in Interlaken) and the author of this article. The aim was to coordinate activities on molecular modeling and molecular simulations in German-speaking countries and to organize meetings on specific topics in a similar manner as is the tradition in Britain.

The 1994 Darmstadt Workshop (May 10–11) is organized for the first time as a meeting of the German-speaking branch of the MGS. The scientific program will be organized by Dr. Tim Clark from the University of Erlangen and Dr. G. Dölz from the Biozentrum in Basel. The general idea of the workshop will not be affected by this change in organization.

- (1) The workshop language will be German, but English presentations are welcome.

- (2) The workshop should, in particular, give young scientists from universities, research centers and industrial companies the chance to present their most recent ideas and to discuss these on a wide platform.
- (3) In principle, all participants are responsible for their own expenses. If money is available, students may have the chance to obtain a refund from the organizers.
- (4) The contributed papers can be expanded on during two keynote lectures given by invited speakers.
- (5) Hardware and software companies are welcome to present their products during the workshop.
- (6) The workshop should take place every year in May on the two days before Ascension Day, in order to combine it with the annual meeting of the Deutsche Bunsengesellschaft für Physikalische Chemie.

However, there are some new details as well.

- (1) The Darmstadt Workshop will be (from 1994 onward) an official meeting of the MGS German-speaking branch organized by the MGS in cooperation with the Institute of Physical Chemistry of the Technical University, Darmstadt.
- (2) It will, at least in the near future, include the annual member assembly of the German-speaking branch.

## REFERENCES

1. *Molecular Modelling—Information Trends* (Bundesministerium fuer Forschung und Technologie, Ed.) BMFT, Bonn, 1988