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Editorial

Reinvention of the *Journal of Molecular Graphics and Modelling*: Defining a Discipline

The original *Journal of Molecular Graphics* (JMG) was founded in 1983 as a result of the formation of the Molecular Graphics Society (MGS) in the UK. The MGS arose because of the rapid development of new computing and graphics technology which allowed scientists to explore relationships between the structure and function of molecules.

In the early 1980s, the term molecular graphics meant more than just visualization methods; it was the mechanism whereby structural analysis, molecular design, databases of experimental information and molecular structure, and computed molecular properties were brought together as a powerful collection of tools for answering chemical and biological questions. The impact of computer graphics was so great that the terms "molecular graphics" and "molecular modelling" were sometimes used interchangeably in the early 1980s. The MGS was established for the promotion of molecular modeling research and to serve as a forum for scientists from backgrounds as disparate as protein structure determination, medicinal chemistry, computational chemistry, and technology innovation, all undergirded by computer-based methods.

The JMG was initially edited by Andy Morffew of IBM (UK), but from mid-1984 it was led by Graham Richards with Vivian Cody as US Associate Editor. The journal proved to be an effective forum for reporting relevant algorithms and applications. However, during the 1990s, a number of developments impacted the journal. A subtle but steady change occurred in how the term "molecular graphics" became increasingly viewed as limited to visualization techniques. To counter this, the MGS changed its name to the Molecular Graphics and Modelling Society (MGMS), reflecting its genesis but importantly the ongoing core interests of its members.

In 1997, Graham Richard stood down as editor of the journal (see editorial in Vol. 15, No. 1), and Rod Hubbard was appointed by the MGMS. He has overseen a change in the name of the journal and, in collaboration with the publishers Elsevier Science, recruited the Computers in Chemistry (COMP) division of the American Chemical Society (ACS) as an equal partner in promoting the journal.

The ACS COMP division was started in 1974. Its 25th anniversary will be celebrated in 1999. The truly broad scope envisioned for the division is indicated in the original mission statement as recorded by the first chairman, Peter Lykos: "Through symposia, programs and other means provides a forum for academia, government, and industry to discuss and extend the large and growing impact of computer technology on all of chemistry; constitutes an interface between chemistry and computer science, mathematics, statistics, and engineering; examines computer, communication, servosensor and display hardware-software systems in areas such as real-time data acquisition and control, chemical system modeling and simulation of bulk matter from an atomic and molecular perspective including quantum chemistry, computer-aided visualization and correlation of chemical structures with synthesis design, biological activity, etc., chemical data analyses including pattern recognition, information storage and retrieval, teaching chemistry and chemical engineering and the managing of all chemistry-based endeavors."

Molecular modelling and the other potential interests of computational chemists no longer need as detailed an explanation as in this 25-year-old statement because now the scope and usefulness of computational chemistry are widely appreciated and understood by our colleagues in the other disciplines of molecular science. Yet the spirit of the early statement still rings true today.

COMP has grown to a large and robust organization. Currently, it has about 2200 members. The Executive Committee of COMP saw the need to have a journal dedicated to the membership. Over the years, the committee and other computational chemists in the ACS membership tried to interest the decision makers in the ACS publications department in having a journal devoted to computational chemistry, but without success. Hence when the possibility arose of a joint venture whereby the *Journal of Molecular Graphics and Modelling* could be associated with both MGMS and COMP, the COMP Executive Committee enthusiastically entered the current arrangement with Elsevier Science. At the spring 1998 ACS national meeting, the Executive Committee elected Don Boyd to be their editorial representative as co-editor.

Although there are other journals targeting more or less the same audience, JMGM is unique in having the strength of two large professional societies, MGMS and COMP, behind it. Members of these organizations are some of the most well-known and productive researchers in the field. MGMS has frequent scientific meetings, while the semiannual ACS national meetings have seen the necessity for multiple concurrent COMP sessions to handle all the papers being presented.

As the new editors, we are embarking on the process of relaunching the journal to bring it to the forefront of current

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molecular modelling research. We envision the new journal covering all facets of computational chemistry, embracing all the work of today's computational molecular scientists in organic, inorganic, biological, medicinal, analytical, materials, and informatics research. To support this vision, we have appointed a new, enlarged international editorial board with expertise in the many aspects and applications of molecular modelling.

Elsevier Science, our publisher, is doing what it takes to produce a competitive journal. An electronic version of the articles will be posted on ChemWeb, http://ChemWeb.com/. In addition, we are making plans to extend the scope of the Chemical Design Automation News section of the journal to include perspectives and reviews, alongside the current meeting reports and latest announcements of interest to practicing molecular modellers and computational chemists.

We intend to work hand-in-hand with our respected professional societies and with the wider community of computational molecular scientists to create a journal to meet their needs as we enter a new millennium. We hope that you will submit your best work to JMGM and support us in developing a premier journal that defines our discipline.

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Editors, *Journal of Molecular Graphics and Modelling*