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# The Journal of Molecular Modeling: Impact, Expectations and Experience

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**Abstract.** Experience shows that electronic journals are accepted as long as the quality of the published material is up to the standards of printed journals. Therefore, the aim of an electronic journal is primarily to be a serious scientific publication, and only secondarily an electronic publication. The *Journal of Molecular Modeling*, published for the first time in 1995, is the first fully electronic journal in chemistry. The aim of the journal is to provide high-quality science and take advantage of the electronic format. From the beginning, the journal was designed as trilogy of on-line, CD-ROM, and printed versions, which guarantees longevity of the published research data, allows access to articles and supplementary material without depending on the Internet, and allows the reader to leaf through the journal in the classical fashion. However, this does not mean that the *Journal of Molecular Modeling* will always be published in a conservative 'book-like' format. The goal is to find the electronic format that most appeals to readers without sacrificing the scientific quality of the journal. Scientific journals are steadily developing towards active and interactive publications.

## Introduction

In 1995, the *Journal of Molecular Modeling* was a promising newcomer among the host of chemistry journals [1][2]. What started as an idea at the ACS (American Chemical Society) fall meeting in 1994 developed to become the first fully electronic journal in only a few months. The first hurdle for the pioneer was to convince abstracting and indexing services that an electronic journal is a serious scientific publication. From the beginning, the *Journal of Molecular Modeling* was designed as trilogy of on-line, CD-ROM, and printed versions, which guarantees longevity of the published research data, allows access to articles and supplementary material without depending on the Internet, and gives the possibility to leaf through the journal in the classical fashion.

The aim of the journal is to publish high-quality scientific contributions to the field of molecular modeling in its widest sense. This means that work on methodol-

ogy (from *ab initio* molecular orbital theory to database technology and artificial intelligence techniques) and applications (from pharmaceutical and biological studies through to small molecules, materials, and catalysis) of computer techniques in chemistry are welcome.

One important aspect of the *Journal of Molecular Modeling* that has been emphasized from the beginning is that its 'raison d'être' is to provide high-quality science, not to be an electronic journal [1][3]. The electronic format does, however, give substantial advantages to authors and readers, especially in the molecular modeling field, which relies heavily on color graphics and 3D structures to present results. It was initially agreed that Springer-Verlag, Heidelberg, would print a conventional hard-copy version of the journal and that the now defunct Swiss software company *Megalon* would provide the servers for the publication of the on-line version. Since *Megalon* ceased trading in mid-1995, the journal has been marketed by Springer and made available on Springer servers in Heidelberg and New York.

The *Journal of Molecular Modeling* deliberately adopted a conservative for-



Fig. 1. Layout of a full-paper published in the *Journal of Molecular Modeling*

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mat in its first year of publication. This policy was partly a consequence of the desire to emphasize the scientific quality of the journal rather than its electronic format, but also designed to retain links to the familiar printed journals and to underline the professional publisher's involvement in the design and layout of the papers (Fig. 1).

In the second and third year, considerable technical development in the direction that was originally intended for the journal has taken place. The papers include VRML scenes, video sequences, and 'hypertables' in which molecular structures can be accessed by clicking the appropriate cell of the table [4]. This sort of development necessarily means that there will be an increasing gap between the electronic and the hard-copy editions as the years go by. We are approaching the situation that a fully electronic version of a publication will be accompanied by a more conventional 'print-like' version, but that the two will only have the information they contain in common. This sort of presentation will become standard for electronic media, as we begin to realize that browsing through an electronic journal is a very different process to flipping through pages of a printed edition. It has taken some years of experience to realize that the maximum length of text to be read on a computer screen is 1500 words. On the other hand, nobody is willing to print hundreds of pages on their own printer. The goal is to find the electronic format that most appeals to readers without sacrificing the scientific quality of the journal.

## Features

Table of contents and graphical abstracts of papers published in the *Journal of Molecular Modeling* are freely available on the WWW, either on the Springer servers in Heidelberg (<http://link.springer.de/journals/jmm>) and New York (<http://link.springer-ny.com/journals/jmm>) or at the Computer-Chemie-Zentrum in Erlangen (<http://www.ccc.uni-erlangen.de/jmolmod>) (Fig. 2). The statistics for the Erlangen server, which operated throughout the years, indicate a very wide acceptance of the electronic format of the abstracts. Perhaps surprisingly, the acceptance of the *Journal of Molecular Modeling* is wider among industrial companies (mostly from pharmaceutical and software industries) than from academic organizations. Although individual academics have embraced the concept of the *Journal of Molecular Modeling* enthusiastically,

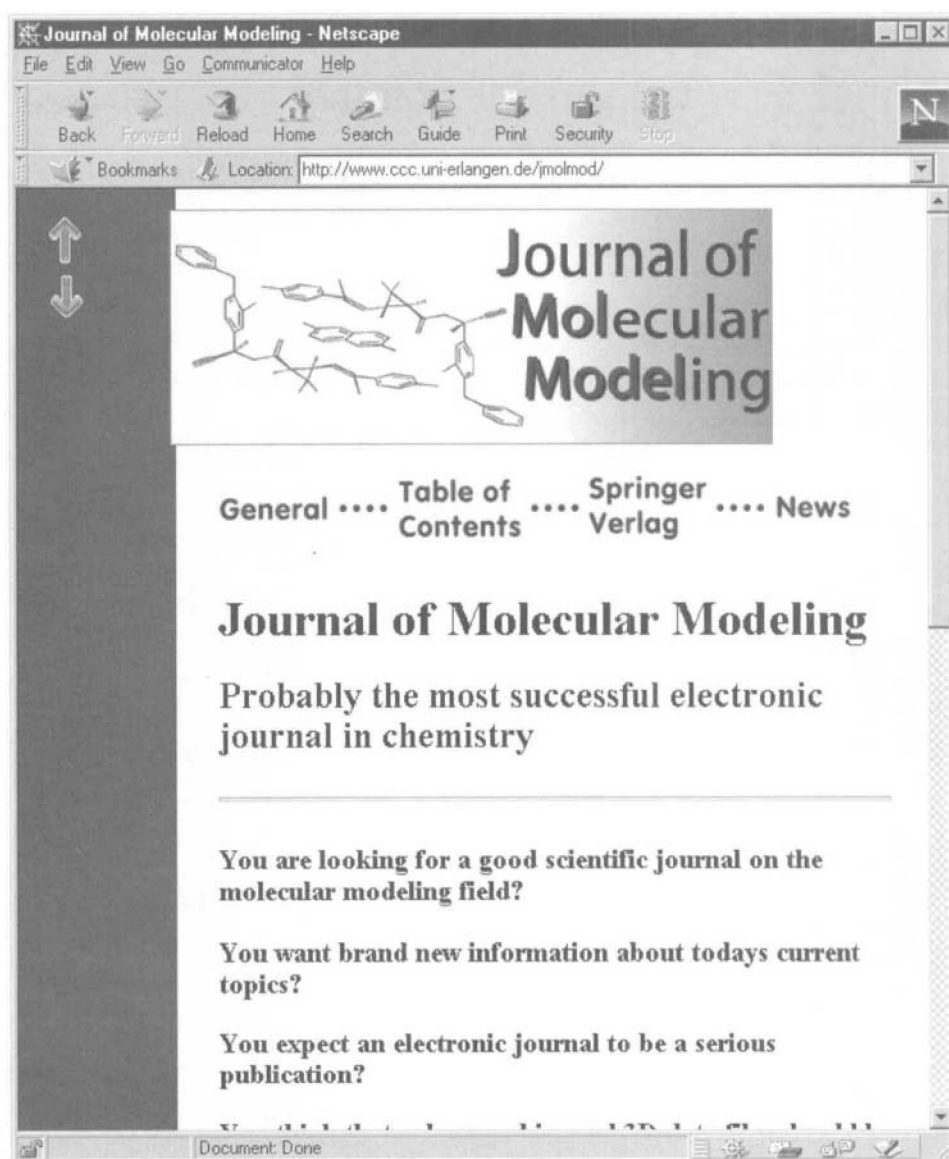


Fig. 2. The journal's homepage at the WWW server of the Computer Chemistry Center (University of Erlangen)

university libraries have been slow to adopt to the new format.

The full text of papers published are available as fully hyperlinked PDF files via the Springer WWW servers. Atomic coordinates and protein structures are given as XYZ or PDB files, which can easily be viewed using Rasmol or any other molecular viewer. Molecular surfaces are generally presented as VRML scenes, and molecular dynamics simulations or reaction coordinates are shown as videos. The ability to view molecular surfaces and reaction mechanisms interactively within the papers is one of the major advantages of the electronic format that has, however, been used only sparingly by authors so far. Similarly, authors have been slow to use the possibility of providing extensive supplementary materials within their papers. Quite generally, authors have tended to submit manuscripts that would also be suitable for a conventional printed paper,

with the difference that the graphics are mostly in color.

The *Journal of Molecular Modeling* was one of the first 100 journals that were made available through the information service LINK in spring 1997. LINK is a new and innovative information concept from the Springer group of companies, which links printed and electronic editions of their journals and books. LINK brings a wide variety of information directly to the desktop of scientists and lecturers, librarians, information brokers, and students. Using Internet technology, LINK is generating an extensive digital marketplace called the 'Forum for Science', organized into scientific libraries such as 'Chemical Science Online Library', 'Medicine Online Library' or 'Physics Online Library' (Fig. 3). One of the most important features of the LINK project is a full and structured search function. Among the categories that can be used for specify-

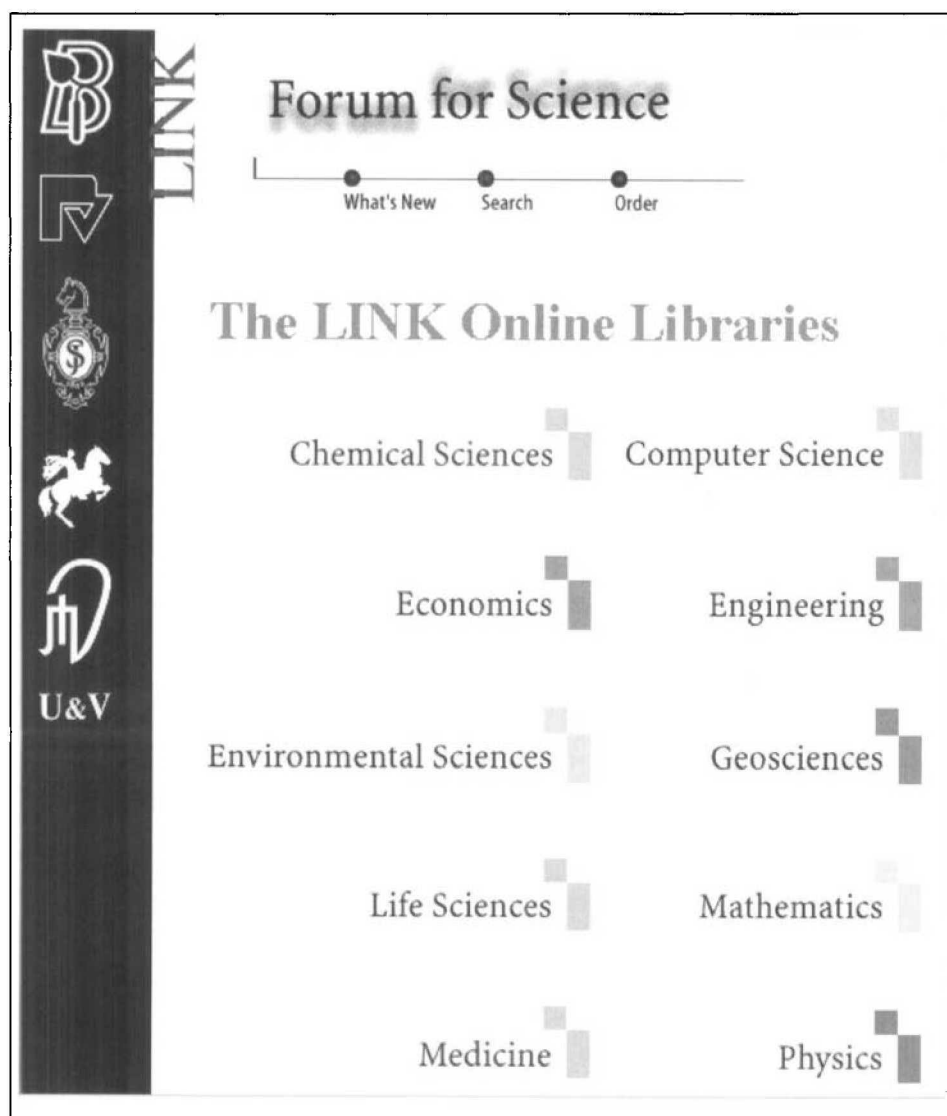


Fig. 3. LINK - Forum for Science

ing a search request are: journal title, date range, title, author, keywords, abstract and full text. A user can insert values for any category. Specifications can be combined with a boolean arguments such as 'and', 'or', 'but not', etc. The result of a search request is a list of hits, containing all articles that match the search conditions. A sophisticated relevance ranking allows the most important articles to be displayed first. Each entry on the hit list contains the following information: author, title of the article, journal name, year, volume, and issue of the paper, and a link to the abstract.

The LINK ALERT service offers readers the possibility to automatically receive the table of contents of journals of interest via e-mail. By subscribing to this service, a user profile is set up. As new material is added to the LINK server, it will be processed against the profiles. Subscribers to the alerting service will be informed by e-mail accordingly.

In 1997, new features were added to the *Journal of Molecular Modeling*. The

immense popularity of the graphical abstracts, which are freely available, has prompted us to offer *Enhanced Abstracts*. *Enhanced Abstracts* are short (up to 6 slides including title slide) HTML slide shows outlining the contents of the full paper. They are intended to allow authors to present a concise picture of the salient points of their paper without the necessity to give hard data or literature references, which are reserved for the full version of the paper. The slides should convey the message of the paper as effectively as possible, much like a conference poster. Generally, relatively little text and as much graphics material as possible are most effective in slide shows of this type. Active objects, such as VRML scenes or atomic coordinates, can also be included in *Enhanced Abstracts* [5].

Also for the first time in 1997, short communications were published within the journal. The *Journal of Molecular Modeling* communications are intended to provide unprecedentedly short publication times for urgent communications of

four printed pages or less. Our aim is to complete the refereeing process (given positive reviewers' comments) within one week, giving a total publication time of 10-18 days. In order to achieve this goal, a web-based refereeing system, in which a panel of referees who have declared their willingness to respond within extremely short time, has been implemented. The referees will be given access to the publication to be reviewed via the Erlangen WWW server. This naturally means that the articles must be submitted electronically in a web-browser-readable form. The final published versions of the *Journal of Molecular Modeling* communications are carefully edited and produced like full papers. Communications may include color graphics or other electronically oriented presentation materials and unlimited supplementary materials.

The third innovation in 1997 was the publication of *Journal of Molecular Modeling* reviews. These reviews of unlimited length on important modeling topics are freely available for three months after the publication date for e-mail comments from other researchers and replies from the authors. The e-mail discussion becomes part of the final published version of the review. We call this kind of publication Review & Open Discussion. In this way, we hope to encourage open and constructive discussion on subjects of current interest.

Every feature added to the *Journal of Molecular Modeling* must fulfill the aim of general and comfortable access to the journal and all of its tools are designed to be used by chemists, rather than Internet specialists.

### Survey - (Electronic) Publishing in Chemistry

During the period from October 1, 1997 to November 13, 1997, a survey was conducted via the WWW. The main topic in question was the publication habits and the general attitude towards electronic publications, both from the view of readers and authors.

The answers came from scientists all over the world. A total of 406 replies. 23.2% were sent from Germany, followed by the USA and the UK. 30% of the participants are professors, 26.8% stated that they have a position in industry. Most of them are doing research and regularly write and read scientific papers. All of them use e-mail and WWW at their daily job. Surprisingly high is the percentage of authors (65.3%) that write their articles

directly on the computer. Only 3.1% write their articles by hand before copying them to the computer.

There is a great demand for an inexpensive way to publish color graphics. The presentation of atomic coordinates and 3D structure files followed in second place. 25% of the participants would like to include videos in their publications. Refereed journals are the most common address to submit manuscripts, which was chosen by 85.2% of the authors. Only 5.7% have already submitted a contribution to an electronic conference or plan to do so. The most important selection criteria when choosing a journal are reputation and coverage.

78.4% of the participants would considerate submitting a manuscript to an electronic journal as long as the scientific value is granted. Citability and the archival of published material are a great concern. Reasons for not submitting papers to an electronic journals are copyright, accessibility and impact, quality assurance, and, psychologically speaking, the scientific value is rated lower.

When asked about the impact that electronic publication will have on the printed media, 35.7% of the participants answered that they think (or wish) that printed publications will remain the most important reference work. 27.6% responded that electronic publications will promote the use of printed material, and 25.4% stated that electronic publications will replace print. For handbooks, dictionaries, references, and numerical information, electronic media will play an important role. The impact of electronic conferences is rated much lower, the reason being that on-line conferences will not replace the critical face-to-face interaction of traditional meetings.

### The Libraries

Four years ago, librarians were reluctant to accept that the world of science publishing is changing. The advent of electronic publishing has created concern among both publishers and librarians, despite its distinct advantages over print in terms of delivery time, additional features, and flexibility. Higher subscription costs, licensing agreements for access, and the uncertainty of archiving have all been sources of increasing tension between academic publishers and their customers [6].

In the beginning, the infrastructure at the libraries was simply not there. They had no possibility to access on-line jour-

nals and ergo did not know how to handle them. Industrial libraries, mostly from pharmaceutical and software companies, have shown the advantage of for-profit enterprises when it comes to responding quickly to new circumstances and needs. They were among the first subscribers of the *Journal of Molecular Modeling*.

With the breakthrough of the WWW, the librarians discovered the net as a fruitful information source. They started to use the Internet in their daily work. This does not mean that users of a library have direct and unlimited access to on-line journals. In many cases, libraries deliver printouts of electronic articles, meaning that information-enhanced papers cannot be delivered to the reader (scientist) without loss of information. In the case of the *Journal of Molecular Modeling*, this problem is now circumvented through the availability of the journal within the *Springer LINK* project. Papers published on the LINK server can be accessed directly from every computer within the domain of the subscribing library. The problem is that libraries often do not have the funds to pay additional money for electronic access. The scholarly communication crisis has resulted from the long-term willingness of the libraries to spend huge amounts of money on science journal subscriptions. The Web gives us the illusion that we can get all the information we need free of charge. Voices are raising asking for a preprint service in chemistry following the <http://xxx.lanl.gov> model that was set up by the physics community. But in a world where data enters the records directly from the source, no information is given about the quality of the accessible material. We have to get used to the idea that we have to pay for information, not for the paper it is printed on.

Another issue that is often discussed is the ownership of access to information even after cancellation of a subscription. Or just the long-term access to the published material, as nobody knows for how long articles will be accessible at the publisher's site. Some services promise nothing, some offer service in perpetuity at no charge, and some are developing cost models for the access fee portion of historically owned on-line materials after cancellation. Of course, there are archive support costs involved in each of these scenarios.

### Outlook

The experience shows that electronic journals are accepted as long as the quality

of the published material is up to the standards of printed journals. Therefore, the aim of an electronic journals must be to be a serious scientific publication first, an electronic publication second. The quality of a journal depends heavily on peer reviewing and quality assurance throughout the production process. The publication times can only be shortened by implementing as much electronic processes as possible.

In the beginning, sophisticated presentation materials like 3D coordinates, movies, and VRML scenes have been used sparingly by the authors. With the growth of the WWW and the development of the corresponding tools, the use of multimedia elements in publication has become more and more common. Today, the editorial office of the *Journal of Molecular Modeling* rarely receives a paper that does not have some kind of supplementary materials, the publication of 3D coordinates is now standard routine. In the future more and more hypermedia elements will be included in the publications of the *Journal of Molecular Modeling*. The format of articles will some days be that of a hyperlinked slide show and annotation can be added directly to the electronic document. Scientific journals are developing to be more and more an active and interactive publication.

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