
## Mathub.com: Computational Methods in Materials Science

The website mathub.com was launched early last year and defines itself as "the focal point for computational materials science on the web, providing a gateway to scientific information about modeling and informatics". The contents of this site is free, but password protected. Hence, before it can be accessed, the user needs to register name, organization, and also the area of scientific interest. As the .com indicates, the mathub site has a commercial background and is actually run by MSI Inc., one of the major providers of modeling software for life and materials science research. However, there are hardly any direct references to this relation. Rather, mathub.com tries to establish itself as an independent, non-commercial platform, and the connection to MSI is mostly documented only indirectly by the large amount of MSI-related information presented on the pages. As in many similar cases, one asks oneself why these pages need a registration and what MSI has in mind with the personal information of its registered users, of which there are around 1500 up to now.


Figure 1. Industry page in www.mathub.com

There are two main areas accessible from the mathub.com homepage, namely "reference" and "magazine". Under "reference" a large amount of useful information can be found. There are pages describing the fields of materials modeling and materials informatics. Hyperlinks to selected application areas and explicit examples of where computational materials science is of relevance provide further information, including many hyperlinks to sites outside the mathub domain. A number of pages is devoted to the use of molecular modeling in education including a small and, hence, incomplete list of universities that offer courses in computational chemistry and molecular modeling. More interesting is the compilation of references to some of the existing online courses on this subject.

A large fraction of the "reference" part deals with the "history of modeling". Actually, under this category one not only finds an interesting historical review on the development of the various computational methods in chemistry, but also articles describing the history of chemistry in general. In addition, a brief history of computing is presented. Particularly interesting is the survey of the history of commercial software houses in computational chemistry and the corresponding mergers and alliances that have happened during the past 20 years or so. One also finds a report on the "molecular modeling community" with references to the appropriate divisions of the ACS and the Royal Society of Chemistry (a link to the Computers and Chemistry division of the GDCh is unfortunately missing) and to the most relevant journals in the field (for some reason the Journal of Computational Chemistry did not make it into this list). Another section deals with the "scientific theory", i.e., the theoretical backgrounds of computational chemistry. While there are entries for many relevant items, from "molecular graphics", to "mesoscale modeling", only little and fairly superficial information is actually given. Exceptions are articles on density functional theory and some other quantum chemical approaches. A glossary of terms relating to molecular modeling completes this section. While this is a useful feature, the explanations and definitions given tend to oversimplify things.

Finally, the "reference" part offers a "software directory", with an extended hyperlink collection to free and commercial software from various vendors for many applications, and a section on "scientific references", which contains hyperlinks to many important chemistry journals and a searchable database with over 1500 computational materials science references.

The "magazine" part of the web site contains—as the name suggests—contributions on several topics of interest to computational chemistry in general and the materials modeling community in particular. At the time of writing, among the articles is a report adapted from the Financial Times on the growing role of computational chemistry in different sectors of the chemical industry and a feature article on COSMOlogic, a small computational chemistry start-up company. In addition, there are reviews of books and web sites relating to molecular modeling, lists of conferences and vacancies in academia and industry, and other important and not so important, but entertaining, information related to materials science and molecular modeling.

In conclusion, mathub.com is an interesting and, as it seems, well maintained entry point into web resources not only relating to the special field of computational materials science, but to computational chemistry and molecular modeling in general. The information provided is mainly at the non-expert level, but also the specialist will find interesting links and references. Whether mathub.com will actually be able to fulfill its ambitious goal of becoming the major portal of computational materials science remains to be seen. In any case, for those interested in computational chemistry, this site is worth a visit.

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