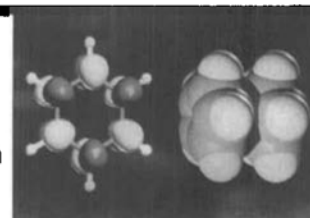


COMPUTATIONAL CHEMISTRY COLUMN

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Computational Chemistry: What Does Industry Expect from Academia?

The question may sound both somewhat vague and a little naive. But nevertheless, we suspect there are a lot of unspoken, maybe even unconscious, expectations on both sides, the 'Industry' and 'Academia', and in this column we try to analyze what the present position and value of Computational Chemistry in Industry is, what its potential in future may be, and work out what the expectations of Industry are with respect to Academia.

Computational Chemistry in an embryonic state has first found its way into industrial research, particularly into pharmaceutical industry, some 25 years ago through analytical chemistry, and in particular through X-ray crystallography. It was one of the first experiences of chemical research in Industry with 'computers', and in a way with 'Computational Chemistry'. The 3D-structure determination of bioactive compounds, or analogues, by X-ray analysis led quite naturally to questions like 'what is so particular in the 3D-structure of this molecule to make it biologically active?'. As more and more crystal structures were solved, questions of this type were asked more often, and in the late seventies, the need for more intensive studies of this general problem of 'structure-activity relationships' was realized, and 'Molecular Modelling' was born. It is certainly not a coincidence that at the same time quite powerful computer and computer graphics systems were becoming affordable on a departmental level. Out of the initial Molecular Modelling, mostly done in industrial laboratories, grew a respectable new discipline, soon called 'Computational Chemistry' which today has its foundations firmly established, in both Industry and

Academia. A large range of methods and techniques including quantum chemical calculations, molecular model building, simulations of molecular systems, determination and visualisation of complex molecular structures, retrieval of selected patterns in 3D-data bases, *etc.* are applied to all sorts of problems, and an arsenal of computational resources ranging from the PC over the workstations to the supercomputer are used in many laboratories.

One of the main themes of Computational Chemistry is the prediction of material properties from theoretical calculations. While the 'original' problem of 'structure - activity' in biological context is still a major part of the Computational Chemistry world, it has gone far beyond that and has extended into polymer research, catalysis, and into many other areas of chemistry.

What has Computational Chemistry achieved in the last ten years? How many predictions have been made by Computational Chemistry, how many were correct, how many relevant? It is undoubtedly beyond the scope of this column to analyze such achievements, and the reader has probably his own opinion about it. However, accepting for the purpose of this discussion that 'some' achievements have been made by Computational Chemistry, we can then turn to the question on how the 'value' of Computational Chemistry is looked at in Industry and Academia:

For example in industrial medicinal research (and what follows applies similarly to other industrial research), the 'value' of Computational Chemistry is weighed by its

power to predict and design bioactive compounds. The motivation to support Computational Chemistry groups depends on two expectations of research management: *i)* many expensive experiments, *i.e.* chemical syntheses and biological tests, can be avoided thanks to theoretical predictions of possibly active or inactive compounds, in other words, it saves money and time, *ii)* the Computational Chemistry methods give detailed insight into drug - receptor interactions which allows the design of better drugs, and hence gives a competitive edge. The weights of these two factors will probably increase in the next ten years given that both the Computational Chemistry methods and the performance of computational equipment improve in the next ten years at about the same rate we had in the last ten years. The example of pharmaceutical industry probably reflects the situation in other areas of chemical industry as well, and it may well be that survival of many companies - and possibly also the future of tomorrow's chemists - will critically depend on skill and use in Computational Chemistry.

In Academia, the weighing of Computational Chemistry is naturally quite different, its fundamental and methodological aspects being more important, and its practical aspects therefore less emphasized. The main purpose of academic research in Computational Chemistry is the expansion of its predictive power. As such, it has found its way into many Universities, however, in most cases still as a somewhat exotic special branch, tucked away in an 'ivory tower', known only to insiders.

In summary then, it is quite clear what the expectations of Industry with respect to Computational Chemistry in academia are: 'Computational Chemistry should become an integral part of the chemistry curriculum in Universities, not just a specialized branch. In addition, as research and teaching are inseparable duties of academia, laboratories of Computational Chemistry should be integrated into chemistry departments, its teaching and application in chemistry be enhanced and brought to all chemistry students.' In this respect, two Swiss universities and the ETH-Zürich have already started on the way towards such integration of Computational Chemistry; however, much is still left to do, and it is hoped that the example of the three will be followed by the others.