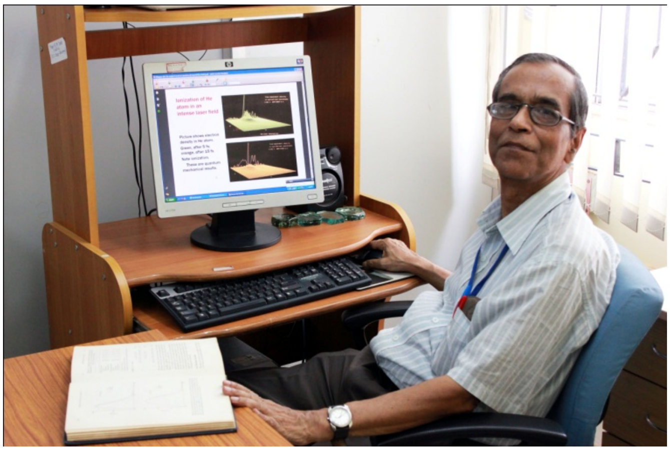
Bidyendu Mohan Deb



B. M. Deb (Photo credit: Subhajit Bandyopadhyay)

Bidyendu Mohan Deb is a Visiting Professor at the Indian Institute of Science Education and Research, Kolkata. His areas of scientific interests have been theoretical chemistry (including the development of original concepts and formalisms, followed by development of sophisticated algorithms and computer codes for accurate demonstration of the validity of the proposed equations), and theoretical atomic and molecular physics. Deb is a chemist with a Ph D in mathematics. He has been keen in developing chemistry curricula in Indian universities and also worked for developing comprehensive science curricula in the country.

Looking back, Deb says he is convinced that his teachers, right from high school to the doctoral level, were instrumental in charting his professional life. In an interview with *Current Science*, Deb recalled an incident that helped define the course of his research years ago – an article he had written for students and teachers was published after a long struggle, following which he received letters from scientists belonging to various disciplines. One of them was Richard P. Feynman, who not only praised Deb's article, but also suggested that he look into stresses in molecules.

How has the field of theoretical and computational chemistry evolved over the years?

Theoretical chemistry has been operating at the interface between chemistry, physics, biology, mathematics and computational science. It deals with systems and phenomena concerning these large subjects. Computational chemistry has been primarily concerned with the development and application of computer software, using theoretical chemistry methodologies, utilizing numerical methods and computer programming in a significant way.

Nowadays not all theoretical chemists and computational chemists develop their own codes. Only some do, if necessary, whereas others employ standard and/or commercially available software packages for performing computations on electronic structure, geometry, various chemical, physical and biological properties as well as various kinds of classical and semi-classical simulations of structures and dynamics of large molecular systems such as proteins, polymers and liquids. Since the 1930s, theoretical and computational chemists have been a major driving force behind developments in computational sciences, including both computer hardware and software development, especially number crunching and graphics. Graphics is particularly important because chemists find it difficult to work without detailed visualization.

Because of their subject's complex, multidisciplinary nature, theoretical chemists have been somewhat like orphans! You can find them everywhere, in chemistry, biochemistry, physics, mathematics, computer science, chemical engineering, materials science and engineering departments as well as in industries across the world, though I believe very few, if any at all, in Indian industries. Since earth scientists are currently using theoretical chemistry computations for interpretations of their data, perhaps we will soon have a theoretical chemist in an earth science department! Historically, mathematicians, physicists, chemists, computer scientists and even economists have contributed to theoretical chemistry.

What are the interdisciplinary areas that you have worked on?

An interdisciplinary research area that I have pursued is the quantum theory of structures, dynamics, and properties of atoms and molecules. I have had great pleasure in devoting some time over the years for designing exciting and colourful chemical experiments, based on research literature, for undergraduate and postgraduate teaching laboratories. Each of these brings as many sciences as possible on the common platform of one single experiment.

This was to partly satisfy my hunger for experimental chemistry. Also, writing on integrated learning in sciences, designing new curricula and developing new courses have been something of a passion.

What do you see as things that have changed in the field of chemistry, especially theoretical chemistry and computational chemistry?

I see considerable development in the interfaces between chemistry and biology as well as chemistry and materials science. Some developments have also occurred in the interface between chemistry and earth science. With the advent of improved computer hardware and software, the way chemistry used to be done has changed, in the way data are recorded and analysed. Computational chemistry software packages are being used almost routinely by many experimental chemists. Computational chemists are themselves using standard software packages to tackle more and more exciting and challenging problems. Two- and three-dimensional visualizations (graphics) are increasingly being employed. Experimentally, attempts are being made to probe single molecules rather than molecules in an assembly. Combinatorial chemistry as well as green chemistry have been in existence for some time. A synthesis protocol utilizing artificial intelligence also exists. Attosecond (10^{-18} s) phenomena, concerned with electronic motions, have emerged very recently. Overall, I sense a great churning taking place in chemistry.

What do you think lies in the future for theoretical chemistry and computational chemistry?

If I am not wrong, of the total global population of theoretical and computational chemists, 90% or even more are computational chemists. Two things ought to be noted here. Software packages represent the technology of theoretical chemistry and they employ existing theories which cannot be regarded as 'perfect'. Everybody knows that 'all exact sciences are dominated by approximations'. Chemical systems being highly complex, it would be rather unrealistic to play with toy models which admit analytical solutions. Therefore, the need for developing new concepts for improving existing theories would remain strong because this is an open-ended quest. Needless to say, software packages should not be used as 'black boxes'.

In India, the number of theoretical chemists who can traverse the whole gamut of theoretical chemistry, viz., generation of concepts, formalisms, algorithms, computer codes and new ways of interpreting computed numbers, can be counted on only one hand. Most of them are in their fifties and sixties. The prospects of replenishments occurring through bright, imaginative and capable young chemists appear bleak.

How has computation changed the way research in chemistry is carried out?

Over the years, there has been a sea change in the attitude of chemists. Earlier, any theoretical method and the numbers computed from it had to be justified by comparing with experimental results. This has drastically changed because of two reasons. First, the sophistication in theory, algorithms and computer codes is now so good that these frequently deliver computed numbers much beyond present-day experimental accuracy. Second, there are many situations in which it is extremely difficult to perform an experiment, e.g. to study a very short-lived molecule or study a phenomenon such as the folding of a protein in a biological environment. Theoretical and computational chemistry could be the only route to take in such cases.

With the availability of dependable and commercially available software packages, developed by theoretical and computational chemists, in collaboration with experts in numerical analysis and methods, an interesting situation has come about. The synthesis and structure of a new molecule discovered in the chemical laboratory is nowadays justified by experimentalists by doing a geometry optimization according to a good software package. On the other hand, the experimental determination of structure generally resorts to a combination of methods.

Where do you think physical chemistry stands relative to other areas like inorganic and organic chemistry?

Since my undergraduate days, I have been acutely uncomfortable with the attitude that chemistry can be completely classified into inorganic, organic and physical chemistry. These are artificial intellectual barriers. The numbers of researchers and publications in certain areas of chemistry have been steadily increasing and will continue to do so. In terms of the number of researchers in various areas, there has been a seriously lopsided development in our country because of the tripartite classification. One hears of cases where there is a large number of Ph D students with just one supervisor. I hope the situation will improve and a balanced development will take place. Until 1960s, successive Nobel Committees apparently did not find theoretical chemists worthy of the Nobel Prize, although they had enormous impact on the whole of chemistry. That also changed from the 1960s. Of late, even a theoretical condensed matter physicist has received the Nobel Prize in chemistry. So, the earlier we teach ourselves to climb over these barriers, the better it is for the growth of chemistry. I would be very happy to see a Nobel Prize in chemistry from India, for work done in India. I think this is overdue.

How are physical chemistry and chemical physics different from each other?

Since both the terms refer to the interface between chemistry and physics, they should have the same meaning. However, in usage this is not so. The term 'chemical physics' was coined in the post-quantum mechanical era and popularized by journals in chemical physics. One might simplistically say that if in the chemistry–physics interface one is veering more towards chemistry then one is doing physical chemistry, whereas if one veers more towards physics one is doing chemical physics. Alternatively, since science develops by progressive quantification, one might say that chemical physics is the modern, more quantified version of physical chemistry. But, I think all such distinctions are somewhat contrived. However, chemical physics has certainly been enriched by contributions from many physicists who probably felt more comfortable with this term than 'physical chemistry'. It may be worth noting here that an 'over-zealous' scientist had once defined physical chemistry as 'the study of everything that is interesting'!

What would you like to see changing about the way chemistry is pursued?

Within the global scenario, I believe we are not too bad in dealing with problems of fundamental importance in chemistry. However, I would like to see much greater intensity here, in terms of issues that are not being tackled in other countries. Our young researchers need to quickly come out of their postdoctoral experience and move into original lines of thinking of their own. Funding agencies should support ambitious projects from our young chemists and not treat them with skepticism. Where I would like to see extensive leap-frogging is in the development of new and sophisticated technologies born in chemical research laboratories, in collaboration with other scientists and engineers, wherever necessary. Some examples could be attosecond and X-ray lasers, a working quantum computer, new drug molecules by drastically cutting down the laboratory-to-market time schedule through a clever but absolutely safe multidisciplinary approach, etc. The list is quite long. Sophisticated chemical technologies that would be inexpensive and ecofriendly, and can improve the lives of common people, especially those in rural areas, need to be developed as quickly as possible.

You were involved in the development of chemistry curriculum for universities. What are the key aspects of a good chemistry curriculum according to you?

Irrespective of what an individual chemist may practice in his/her own research, a chemistry curriculum must not split chemistry into inorganic, organic and physical chemistry, and there should be no specialization in any of these three up to the Master's level. I strongly believe that this tripartite splitting has done enormous damage to the free development of chemistry in our country. Throughout the Bachelor's and Master's years, there should be self-exploration through as many small and medium projects as possible. Science can be learnt only through a dialogue with nature, through experiments in the laboratory and in natural environments outside the laboratory. Laboratory programmes in our country are in a sad state. We must bring back imagination, excitement and wonder into the laboratory courses in chemistry. This is easier said than done. Here theoretical and computational chemists should join hands with their experimental colleagues in devising concept-oriented, technique-intensive and generally fun experiments for students. We must also bring back experimental demonstrations during classroom lectures. Let us not forget that chemistry is a subject combining magic, logic and aesthetics.

The life-blood of any educational programme is a dedicated and conscientious band of teachers. I would request the teachers concerned in formulating any chemistry curriculum to keep in mind that it is a central science, overlapping with practically any subject under the sun.

What do you think about the teaching of chemistry in schools and colleges?

I am afraid this is rather unsatisfactory, in spite of long and determined efforts by many bodies and many scientists. Almost every school and college in our country has a small group of dedicated teachers in chemistry. Generally, every effort they make for curricular improvement is thwarted by the majority of other teachers, an unresponsive administration as well as state government. One should realize that true democracy does not mean disregarding the voice of the minority by the majority, and one should indeed listen to the voice of conscience.

Classroom teaching of chemistry has tended to emphasize rote learning. Laboratory programmes, without which science cannot be taught and learnt, are in shambles. In the laboratory, students are sometimes encouraged to fudge or even manufacture data instead of doing an experiment honestly. This is extremely depressing because we are corrupting the minds of future generations, which are our only hope.

Because of a combination of such factors and a perceived lack of intellectual challenge, bright students have tended to move away from chemistry. But dedicated teachers should keep on struggling, as many of us have been doing over the years and the situation is bound to improve.

What kind of prospects do young theoretical and computational chemists have in India?

Many years ago, we said that every chemistry department in Indian colleges and universities should appoint at least one theoretical and computational chemist. In universities, the critical number would be three. Because of the multidisciplinary nature of the subject, a theoretical chemist can teach quite a few areas and would therefore lend strength to the teaching programmes. Unfortunately, decades have passed and still this hasn't happened. Secondly, in sharp contrast to industries elsewhere, Indian industries by and large have not felt the need to appoint theoretical and computational chemists. All these have drastically reduced the employability of young theoretical and computational chemists, who show enormous personal courage to go into these areas. As a result, theoretical and computational chemists have found employment only in a few national institutions. I find this overall situation unfair, unjust and fraught with danger for the future development of chemistry in India.

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