Bidyendu Mohan Deb

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.

Excerpts from his interview*

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.

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.

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 has not 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 institutes. I find this overall situation unfair, unjust and fraught with danger for the future development of chemistry in India.

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.

*The full version of the interview can be found at: 25 Jan 2012/165a.pdf.

Richa Malhotra