BARC Q&A

Tête-à-tête with

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*Dr. Niharendu Choudhury**: **You were instrumental in synergizing Theoretical Chemistry Community in BARC. Starting your journey as a training school graduate in Heavy Water Division (HWD), which was not a pure basic research division, how did you establish yourself amongst the ranks of the most renowned theoretical chemists in the country? What were the significant challenges and opportunities during your journey in BARC?**

Dr. Swapan K. Ghosh: Thank you for your kind invitation and positive words. Earlier, there was a theoretical chemistry community, with several excellent scientists (mostly physicists) nurtured by Dr. P. G. Khubchandani, who were pursuing theoretical research, covering diversified areas such as formalism development, work on molecular orbitals, issues related to solid state physics, etc. Many of these scientists were my teachers in the BARC training school, and have provided encouragement and inspiration to me.

After graduating from the BARC training school, I joined the Heavy Water Division (HWD), where there was a need for theoretical calculation of separation factors in deuterium isotope exchange reactions, in addition to the need for understanding the chemistry of corrosion behavior of components used in heavy water plants. It was great pleasure to work on some of the teething problems faced by heavy water plants of that time and also to carry out theoretical investigations on various existing as well as new possible deuterium exchange reactions for the future. There was good camaraderie among the colleagues, all of whom were geared up to problem solving mode. The work although didn't belong to basic research as such but the work I was involved in (both theoretical and experimental) was the need of the hour and working on them gave me ample satisfaction.

Gradually, I drifted towards theoretical chemistry research riding on the support extended by senior colleagues of HWD. I soon completed my Ph.D. from IIT Bombay under the supervision of Prof. Bidyendu Mohan Deb, an eminent theoretical chemist, followed by post-doctoral research with Prof. Robert Parr in USA, and later came back and started almost full time theoretical chemistry research in HWD on density based theories. Support for my work came not only from my Division Head, Mr. H. K. Sadhukhan but also from the then BARC Director Dr. R. Chidambaram. I was instrumental in developing a computer code (published as a BARC Report) for calculation (based on a density based parametric equation) of thermodynamic as well as transport properties of heavy water at any given temperature and pressure, which proved quite useful to several scientists of BARC and DAE.

Due to strong support to my activities from senior colleagues from BARC, all major challenges proved to be almost surmountable. The opportunities that came in my way stem from the faith the seniors had in my capabilities; and the ensuing journey was quite smooth besotted with minor ups and downs, as is the case most of the time. Gradually, a research group,focusing on theoretical approach, nucleated in HWD, with a few very talented young people who joined us from the ranks of BARC training school. In summary, the BARC system played a positive role in

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Dr. Swapan K. Ghosh

supporting my endeavors in theoretical chemistry research besides transforming me into what I am today. I am truly grateful to BARC and DAE system for that.

Dr. Niharendu Choudhury: **From being a young scientist in HWD, BARC, you have resurrected a full-fledged Theoretical Chemistry Section and later an independent Section. In fact, you were instrumental in establishing a thriving theoretical chemistry community beyond the theoretical chemistry section in BARC. Elucidate the challenges you might have faced in this journey?**

Dr. Swapan K. Ghosh: My interest in theoretical chemistry emanated from the excellent academic teaching by Prof S.C. Rakshit in quantum chemistry in the M.Sc. Class at the University of Burdwan, West Bengal. Additionally, I consider myself fortunate enough to have got an opportunity to work in a thriving atmosphere prevalent in BARC.

I had developed a passion for theoretical chemistry and strongly believed that if one is passionate and poised to work hard, success beckons him. However, I also felt that if one would like to pursue research in a subject more vigorously and fruitfully, the first requisite is to convince oneself as well as others who provide support to this research. Along with me, most of my senior colleagues believed that theoretical research is an integral part of multi-diversified scientific research.

The next challenge is that one needs to have sustained scientific interactions for which there should be a good research team of like-minded people. I started teaching in the Training School quite early in my career and was able to inspire a few very talented young people from the training school to join us. Thus, a research team of theoretical chemistry took shape in HWD. I am extremely thankful to Dr. R. M. Iyer, Dr. J.P. Mittal, Dr. C. Manohar and Mr. H.K. Sadhukhan.

Mr. Alok Samanta, who had a keen interest in mathematics and chemistry at the fundamental theoretical level, was the first to join us from the ranks of training school. He is not only very highly gifted and brilliant but is also an excellent human being who had been admired for his selfless and extremely helpful nature. Mr. Tapan Ghanty, Mr. Chandra Patra and Mr. Niharendu Choudhury joined our team one after the other. All of them have worked on different research problems and have established themselves in their respective fields. This helped us immensely to take up more responsibilities, and address diverse challenging research problems.

Subsequently, we moved to the chemistry group, where the formal theoretical chemistry section was formed with the help of Dr. J. P. Mittal, and also later as an independent section by the then Director of BARC Dr. Srikumar Banerjee. Two more colleagues, Dr. Tusar Bandyopadhyay and Dr. Dilip Maity, who were in the chemistry division initially, also joined us. Dr. Chandrakumar, followed by Dr. Mahesh, Dr. Malaya, Dr. Sajeev and later Dr. Tijo joined us through KSKRA. Three more persons from the training school joined the team - Mr. K. Srinivasu, Mr. Brindaban Modak - and later Dr. Arup Pathak. The team was thus enlarged, and the research areas were also diversified, •••

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Dr. Swapan K. Ghosh

covering problems encompassing quantum as well as classical systems through theoretical approaches spanning over the whole range of microscopic to mesoscopic to macroscopic length scales. Collaboration with experimentalists was also taken up by my colleagues. The help coming from multiple quarters played a vital role in our activities. I have been fortunate to have received whole hearted support and encouragement from Dr. R. Chidambaram, Dr J.P. Mittal, Dr. Srikumar Banerjee, Dr. Tulsi Mukherjee and several others.

Dr. Niharendu Choudhury: **You have superannuated from BARC in 2013, but you are still well aware of the work and the nature of research being carried out in the Theoretical Chemistry Section (TCS), Chemistry Division, BARC.**

(a) How do you compare the research carried out at the Theoretical Chemistry Section with that in other institutes in India and abroad?

Dr. Swapan K. Ghosh: Superannuation is a state of transition that sets into everybody's life, but scientists actually never retire! I keep myself busy in teaching at UM-DAE-CEBS, and also carry out some research (whatever is possible with me). I am grateful to Prof S.M. Chitre and the Chairman, AEC for their support for my association at CEBS. I like reading scientific literature and am fond of being aware of what is going on in my field of research. Moreover, whatever little I could do is due to the help from my colleagues in theoretical chemistry section, and as a result of this, I have cultivated close bonds of friendship with them.

The work being done in TCS is of high quality and is at par with the work of many other research groups in the country and elsewhere. One of the main challenges faced by them is lack of sufficient number of PhD students. This has affected the productivity of TCS in comparison to the faculties in other institutes. However, this can at least partially be compensated by the vibrant research atmosphere created by the presence of so many brilliant scientists of diverse expertise under one umbrella, providing an opportunity of learning from each other through discussion and collaboration.

(b) Do you have suggestions/advices to the members of the Theoretical Chemistry Section for improving the quality of their research and visibility?

Dr. Swapan K. Ghosh: Let me start with the general advice by Peter Medawar "Work on important problems" in his book, Advice to a Young scientist, which is always applicable. The TCS community in BARC is already working on important research problems. Of course, there is always scope for further improvement in everything that people do, and the same is true here as well. The best possible thing is to leave it to individual researchers who are well equipped to ask important questions and find suitable solutions. Fortunately, the support for this freedom is usually made available by the senior colleagues.

Visibility of research to the outside world is not an issue today. In this era of high speed information communication good quality work becomes public in no time, thanks to the media! One can also use online platforms of various

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Dr. Swapan K. Ghosh

forums, websites etc to make their work available to others. The quality of the work is the only important aspect, and in my opinion there is no well formulated recipe, although it is often said that the work should be important enough in some sense to the researcher to generate an honest urge to pursue the work.

Still I would like to mention a few points that might be worth considering for the members of TCS in BARC. The most important challenge the team members (or the leadership) of research groups usually confront is the sustainability of the team. For which, one has to work constantly towards maintaining (i) excellence of work at the intellectual level (which will always be respected), (ii) richness and originality of scientific content of the work, (iii) importance of the questions addressed and the answers generated, (iv) usefulness of the work to the people in the immediate neighborhood, other people in the organization, or the society at large in the long term, and finally, (v) selflessness of the leadership and members of the team (always respected). This is of course my personal view within my limited understanding.

In general, I would like to mention a few things about the advantages of being in BARC. Here, we have a number of highly competent scientists under the same roof, with expertise in different areas, which are often complementary. Thus, collaboration among the scientists within TCS (or even discussion and scientific interaction) and also with others will be very helpful to address problems of more diverse nature and also collective wisdom might generate novel ideas. Particularly, for interdisciplinary research, BARC is an excellent place. Walking an extra mile beyond one's comfort zone might be easier in BARC in comparison to elsewhere. Also this might enlarge one's vision. One can also do self-evaluation through a 'SWOT (Strength, Weakness, Opportunities, and Threat) Analysis' for improvement.

Dr. Niharendu Choudhury: **Of late, a majority of the research groups are shifting towards applications of computational tools in different areas of their research rather than pursuing formalism developments. What is your opinion?**

Dr. Swapan K. Ghosh: Theoretical chemistry research consists of using theoretical and computational tools for addressing scientific problems, and provides rationalization and prediction of results of chemical interest. Undoubtedly, development of new theoretical tools or reformulation and modification of existing formalisms or development of new computational strategies etc. forms an integral part of this research. Similarly, calculation of results through computational means constitute another valuable component. Thus, theory and computation are intertwined and represent two sides of the same coin.

Computation and theoretical insights together can provide a true picture of the reality. Thus, both are equally important to dissect a problem for complete understanding and for arriving at solution to a problem.

To summarize, theoretical research has two wings, one dealing with development of new theoretical tools or computational strategies or even interpretative aspects unifying several

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existing approaches, while the other dealing with generating new data through computation, which can be compared with experimental results, if available, or can be interpreted using existing or new formalisms. The individual interest or ability usually determines what a person prefers to do.

Dr. Niharendu Choudhury: **What are the different areas of research in DAE in which theoretical and computational chemistry can play a significant role, and what are the future prospects?**

Dr. Swapan K. Ghosh: Theoretical and computational chemistry research has the potential to provide valuable insights and direction to almost any problem related to molecules, and materials and various physico-chemical phenomena. In particular, when experiment is difficult to perform due to requirement of conditions of high temperature, pressure or radioactivity, computational approach is the only practical solution. Analogously, when a few molecular candidates have to be shortlisted from a large set, such as drug design, solvent design etc, computational screening is a very valuable tool and can potentially save a lot of energy and resources. In this sense, theoretical or computational chemistry research can certainly play a significant role by providing valuable inputs in different areas of research in DAE.

In biological research, computational biology is very useful along the lines of computational chemistry. Since many of the biological processes are chemical in nature and therefore computational chemistry tools will be very relevant for use in computational biology.

Computational chemistry based study of soft matter and active matter is also very useful in biology related research. For waste management research, as mentioned before, solvent selection can be done using computational chemistry. Similarly, development of suitable glass system for radioactive waste disposal, theories of glass transition can be studied within the framework of theoretical chemistry. Quite often, need arises for using both microscopic length scale (involving quantum mechanical investigation) and the atomistic length scale (involving classical MD simulation), which necessitates bridging of the length scales, which is an important area of research (multi-scale modeling) in theoretical chemistry/physics.

Catalysis is another important area of research in DAE. The aspects of single atom catalyst, which are of much interest now, can be studied using computational chemistry. The research on hydrogen energy through development of catalyst for water splitting and also hydrogen storage materials can be done using computational chemistry. In materials science, computational chemistry has been of much help through computational design of novel materials with desired properties. Thus, there are many areas of research in DAE which can be enriched by proper use of computational chemistry tools.

Dr. Niharendu Choudhury: **Now-a-days "publish or perish" is the 'mantra' of a successful research career. Therefore, young researchers are focusing on the quantum of publications rather than fundamental developments. How do you look into this.**

Dr. Swapan K. Ghosh: In my opinion, publication is not an objective but a by-product in the sense that it is a vehicle or platform to declare research results, thus making them

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available to the scientific world. If one concentrates on the research problem, asks meaningful and important questions, results (and hence publications) will automatically follow. Of course the outcome is not always linearly dependent on the effort and hence the number of papers may not be uniformly distributed in time. In this regard, DAE has been very considerate by encouraging scientists to take up challenging problems in preference to handling relatively easy problems giving rise to faster publications. Also "Publish or Perish" has never been the prime motivation for BARC, to the best of my knowledge.

Dr. Niharendu Choudhury: **With Artificial Intelligence (AI) and Machine Learning (ML) making rapid strides in Computational Chemistry arena, do you think conventional computational chemistry research methodologies based on quantum and statistical mechanics, becoming redundant?**

Dr. Swapan K. Ghosh: ML and AI are now promising new areas which have pervaded almost all domains of research. A simpler version QSAR (Quantitative Structure Activity Relationship), however, had been well known in the chemical field, where one can predict Properties (Reactivity) of molecules in terms of several structural parameters. ML is a sophisticated and highly versatile version of this, if I am permitted to say so. In general, ML or AI has a bright future ahead in all areas of research. It basically extracts science out of generated data sets, through systematization and essentially bringing order out of chaos. I have very limited expertise and knowledge about this area and hence these are only general comments. Of course, AI can never be able to exceed the power of human intuition or intelligence. Also, ML or AI will never make quantum mechanics or statistical mechanics based approaches redundant. On the other hand, one cannot rule out the possibility of new developments by considering a suitable combination of the theoretical formalisms with some of the concepts behind ML or AI, leading to the emergence of new directions of research.

Dr. Niharendu Choudhury: **What do you envisage about the future of Theoretical and Computational Chemistry in India and abroad in the next 25 years?**

Dr. Swapan K. Ghosh: I am a highly optimistic about an extremely bright future for Theoretical and Computational Chemistry research both in India and abroad. I wish I was younger to witness the growth of these fascinating developments and participate in these during the coming years.

The rapid growth of computational resources with immense computing power as well as the developments of data science, ML or AI based approaches are truly fascinating. Thus, it is very difficult to predict what would be the situation in next 10, 15 or 20 years. There may be a paradigm shift in the overall scenario of research in computational chemistry or physics. But one can definitely say that this field is poised for a much higher momentum, and the predictive ability will be enhanced many-fold, although the understanding level may have a rather slow rise. Also, since more people might be inclined to foray the ML or AI field, efforts towards further development of the conventional theoretical approaches might receive less attention, thus making their growth rather slow.

**Dr. Niharendu Choudhury is currently heading Theoretical Chemistry Section in BARC. Dr. Choudhury specializes in diversified areas of research in theoretical and computational chemistry. He is recipient of DAE Scientific and Technical Excellence Award (2010).*