CURRENT STATUS OF THEORETICAL CHEMISTRY IN INDIA

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ABSTRACT

In spite of nearly 35 years' activity in theoretical chemistry, India is not one of the leading countries in the subject. This report identifies the *strengths* and *weaknesses* of theoretical chemistry research in India, listing various topics in *quantum chemistry* (including *quantum biology*), *statistical mechanics* and *non-equilibrium thermodynamics*, which are either pursued or ought to be pursued. Quantum chemistry is relatively the strongest in our country, while the other two are very weak. The *main* weaknesses in theoretical chemistry are: (a) lack of *original* concepts and mathematical formalisms, and (b) lack of indigeneous large-scale computer programs. The reasons for these are mentioned and the strongest institutions in the country identified. For rapid development of theoretical chemistry in India, 4 *advanced interlinked multi-role* centres of research are proposed, one each for the eastern, western, northern and southern zones. Explicit suggestions are made to improve the teaching of the subject in our universities. Finally, a representative bibliography, consisting mostly of recent papers, is presented.

A satisfactory growth of theoretical chemistry is vital for the overall growth of chemical sciences as well as large areas in physics and biology. With careful marshalling of critical masses, India can rapidly become one of the frontrunners in the subject.

1. INTRODUCTION

At a first glance, it may appear gratifying that, ever since its modest beginning around 1950, theoretical chemistry in India has continued to progress on a slowly ascending curve. However, *in spite of nearly 35 years' activity, India has failed to be one of the leading countries in theoretical chemistry.* It is difficult to identify any seminal paper which has heavily influenced the course of international research in the subject*. In Asia, India lags considerably behind Japan and is marginally ahead of China. However, over the last 5 years, China has made determined and rapid strides in the subject and is likely to leave India behind in the near future. This appears astonishing because Indians are supposed to have a propensity for abstract and imaginative thinking.

There are well-known reasons why theoretical chemistry has not struck firmer roots in the Indian soil. These are, to name a few: inadequate (perhaps improper) treatment of theory in university chemistry teaching with emphasis on rote learning; *horror of the average chemist for mathematics and physics*; lack of understanding of a central spirit in science, namely, *all macroscopic phenomena must be explained in terms of detailed microscopic structure and properties*; incomprehension and unwelcoming attitude to theoretical chemistry in university chemistry departments; neglect of atomic and molecular physics in M.Sc. physics and chemistry curricula; inadequate number of trained and practising theoretical chemists†; intense isolation, and inadequate library and computation facilities for the theoretical chemist; lack of interaction among chemists, physicists and mathematicians; etc.

Nevertheless, this writer firmly believes that if a

* This may also be true about chemical research in our country, in general.

† Very few universities have trained theoretical chemists competent to teach the subject at the M.Sc. level.

determined effort is made now, along the lines suggested at the end of this report, *India can take a quantum leap in theoretical chemistry in the next 5 years*. Relatively speaking, theoretical chemistry does not require a massive investment.

One of the objects of this brief status report is to identify the strengths and weaknesses of theoretical chemistry research in India *vis-a-vis* the international scene. Obviously, for a rapid development of the subject, the areas of strength must be consolidated and the areas of weakness strengthened. Needless to say, a satisfactory growth of theoretical chemistry is vital for the overall growth of chemistry as a basic science in our country. It would also stimulate the growth in large areas of physics and biology, as well as bring about technological innovations through *e.g.* new catalyst design, drug design, new conducting and superconducting materials, etc.

Below, we divide theoretical chemistry into 4 major areas and list the topics of activity under them:

(1) *Quantum chemistry* (atoms, molecules and solids; nuclei may also be included), including *quantum biology* and *quantum pharmacology*.
(2) *Statistical mechanics* (equilibrium and non-equilibrium).
(3) *Non-equilibrium thermodynamics*.
(4) *Mathematical methods in chemistry*.

This classification also indicates the diminishing (top to bottom) importance with which these areas have been regarded by chemists in India. Although the list of topics provided in Section 2 for each area is not exhaustive, it does indicate the topics which are pursued* in India as well as the topics which should be pursued in the coming years. Both *phenomena* to be studied and *methodologies* to be developed are included in the lists†. Section 3 identifies the strengths and weaknesses of theoretical chemistry in India while Section 4 makes a number of recommendations (embracing both research and teaching) for future development. Appendix I gives a cross-sectional bibliography while Appendix II describes a questionnaire.

2. VARIOUS TOPICS UNDER FOUR MAJOR AREAS IN THEORETICAL CHEMISTRY

2.1 *Quantum chemistry*, including *Quantum biology* and *Quantum pharmacology*

2.1.1 New developments in quantum mechanics, perturbation theory* (including large-order perturbation theory), group theory^{PM}, operator theory^{M}, etc.

2.1.2 Many-body/field-theoretic approaches*** in quantum chemistry—cluster expansions, propagators, density matrices, etc.

2.1.3 Single-particle density*** in quantum chemistry—forces in molecules, charge density, momentum density, current density, density-functional theory, X_α method, quantum fluid dynamics (an allied field is solitons* in quantum chemistry).

2.1.4 Electron-atom^{P}, electron-molecule^{P}, atom-atom, atom-molecule*, molecule-molecule collisions; scattering theory***^{P}; classical and semi-classical trajectories in molecular reaction dynamics**; intramolecular dynamics*; reaction pathways and transition states*; statistical methods; Lie algebra; information theory.

2.1.5 Relativistic quantum chemistry*^{P}.

2.1.6 Electric and magnetic properties of atoms and small molecules***; coupled Hartree-Fock theory***^{P}; Sternheimer shielding and antishielding**.

2.1.7 Molecular spectroscopy in absence or presence of external fields—semi-empirical** and *ab initio** calculations of

* In Section 2, a single asterisk indicates that the topic is pursued in India, a double asterisk indicates that considerable work has been done in the topic, while a triple asterisk indicates that the work has received substantial citations in the international literature. Superscript P denotes work done largely in physics departments while superscript M denotes work done largely by mathematicians.

† A 5-page preliminary status report was sent to more than 50 Indian theoretical chemists asking for their opinions and their responses to a questionnaire (see Appendix II). Nearly half of them responded to the questionnaire, some more intensely than others.

electronic, vibrational, esr, nmr, etc. spectra; photon-atom, photon-molecule, etc. collisions; astrophysical molecules.

2.1.8 Computational quantum chemistry—methodologies for various types of large-scale and simulated *ab initio* configuration-interaction calculations; electron correlation**; permutation group, unitary group approaches***P; intermolecular forces**; potential energy surfaces*; model potential and pseudopotential calculations*.

2.1.9 Excited-state chemistry; diabatic states.

2.1.10 Large molecules and solids***P (including both *ab initio*, simulated and semi-empirical calculations**)—polymers; organic conductors and superconductors; various properties and structure-activity relationships; solid-state physics***P and chemistry.

2.1.11 Surfaces and catalysis—surface-adsorbate interaction*; bond making and bond breaking; atomic and molecular clusters; catalyst design; effects of electric and magnetic fields on catalysis.

2.1.12 Multiphoton processes and dynamics in intense fields*—nonlinear optics and related phenomena***P.

2.1.13 Quantum biology*** and quantum pharmacology—conformational analysis (classical and quantal)***; membrane transport**; electrostatic potentials*; drug action*; drug design; biomolecular dynamics.

2.1.14 Qualitative concepts* in binding, structure and reactivity of molecules-molecular mechanics.

2.2 *Statistical Mechanics (equilibrium and non-equilibrium)*

2.2.1 Solitons in dynamics

2.2.2 Polymers and macromolecules*P

2.2.3 Critical phenomena***P; renormalization group*P.

2.2.4 Amorphous solids and thin films*P.

2.2.5 Equilibrium and dynamical structures and properties of liquids***—perturbation theory[P]; potential functions; random phase approximation; equation of state; simulation studies; linear and nonlinear acoustics; liquid metals and alloys; ionic melts and solutions.

2.2.6 Electron liquids; Fermi gas*.

2.3 *Non-Equilibrium Thermodynamics*

2.3.1 Nonlinear dynamics of conservative and dissipative systems**—fluctuations; oscillatory phenomena, coupling; steady states, etc.

2.3.2 Nonlinear fluxes and Onsager reciprocity relations**; symmetry principles in rate processes*.

2.3.3 Theory of dissolution and precipitation potentials**.

2.3.4 Living systems—self organisation and chaos*P.

2.4 *Mathematical Methods in Chemistry*

2.4.1 Catastrophe theory

2.4.2 Queuing theory

2.4.3 Graph theory (*e.g.*, for charting the courses of enzymatic reactions)

2.4.4 Postulational developments and inter-linking of thermodynamics, statistical mechanics, quantum mechanics, functional analysis, etc.

3. STRENGTHS AND WEAKNESSES OF THEORETICAL CHEMISTRY IN INDIA

In Section 2 it was clear that the triple-asterisk topics indicate the areas of greatest strength* (see under Sections 2.1.2, 2.1.3, 2.1.6 and 2.1.13; those under Sections 2.1.4, 2.1.8, 2.1.10 and 2.1.12 have been developed by scientists coming from a physics background). Double-asterisks (see under Sections 2.1.4, 2.1.6, 2.1.7, 2.1.8, 2.1.10 and 2.1.13) denote less strong areas while single- and no-asterisk areas indicate positions of weakness. As already mentioned, the latter areas need to be pursued with greater vigour. In this, lack of adequate manpower is a strong inhibiting factor. *Due to educational and socio-economic*

* This does not always mean that the topic has reached a very high level of international competence.

reasons, there are very few practising theoretical chemists in the country, perhaps no more than 100 in all, with a chemistry background. Of these, only about 40 per cent seem to publish in well-known international journals. Interestingly, no theoretical chemistry group in India has reached a critical mass essential for sustained growth. Thus, *there is a crippling lack of a school or centre of research in the subject*†.

The chemistry or allied departments in the following institutions have small active research groups working on the above topics in theoretical chemistry*:

IITs (QC)	—Bombay, Kanpur, Kharagpur, Madras
Universities (QC, NET, SM)	—Banaras (QC), Calcutta (QC), Delhi (QC), Gorakhpur (NET), Hyderabad (QC), Jadavpur (SM), Madras (QC), Panjab (SM), Pune (QC).
Other Institutions (QC)	—AIIMS (New Delhi), IACS (Calcutta), IISc (Bangalore), NCL (Pune), SINP (Calcutta), TIFR (Bombay).

Of the 4 major areas listed in Section 2, *quantum chemistry is relatively the strongest in India with original front-line work going on in a few areas.* But, *the situation is rather depressing for statistical mechanics and non-equilibrium thermodynamics* which have received very little attention from Indian chemists. Urgent action is called for to revive these areas.

Even for quantum chemistry, the *main weaknesses* of Indian research have been those concerning both the *science* and the *technology* of the subject. In other words, we have been suffering from a lack of (a) *original* concepts and mathematical formalisms, as well as (b) *new* algorithms and indigeneous computer programs for large-scale *ab initio* calculations. Since the seventies, weakness (a) has been partially rectified but the situation is still far from satisfactory. Weakness (b) persists and has become extremely acute in view of tremendous progress made in other countries, although most of the above groups have developed small-scale programs for their individual use. Both aspects (a) and (b) above need separate as well as concerted efforts by the strongest research groups. On the average, a large-scale computer program requires about 25 man-years to develop. At present, there is no such group in India; access to the necessary computing facilities is also not available. Note also that during more than 30 years of research in the subject *only one graduate-level book has been published from India.*

One of the principal reasons for the above weaknesses is the inadequate mathematics and physics background of the Indian theoretical chemist. *Theoretical chemistry is a melting pot of chemists, physicists, biologists and mathematicians.* Unfortunately, such an interaction has rarely occurred in India, with the physicist and the mathematician generally viewing chemistry with distaste. Clearly, a new breed of scientists is needed, with unfettered minds clear of any prejudice.

The interaction between good theory and good experiment in chemistry has also been lacking, by and large, in our country. Experiments, such as those in high-accuracy spectroscopy, which would challenge or broaden the domain of validity of a theory are hardly performed in our country*.

It must be considered tragic that in spite of having the potential to be a leader, India is not among the frontrunners in theoretical chemistry. There is a strong feeling among Indian theoretical chemists that a critical marshalling of forces is *immediately* called for in order to give a

† Note that both Japan and China have set up their own Institutes for theoretical chemistry, at Myodaiji and Changchun respectively. A second Institute, named after Kenichi Fukui may come up soon in Japan.

* QC: Quantum chemistry; SM: Statistical mechanics; NET: Non-equilibrium thermodynamics.

* A case in point is the development of photoelectron spectroscopy in England. Although Indian physicists had been working on the photoelectric effect for years, the spectroscopic implications did not strike them.

sudden strong boost to the subject in our country. This can only be done by setting up at least one internationally reputed *school of research*. For this, a massive investment is not necessary. A sustained and gradually increasing outpouring of high-quality work, in the forms of research articles, books, etc. is urgently required.

4. RECOMMENDATIONS FOR THE FUTURE

4.1 Every university chemistry department must appoint at least one *trained and practising* theoretical chemist capable of developing M.Sc. and Ph.D. level courses. Adequate library facilities and research grant must be provided for him. A good theoretical chemist rapidly enhances the reputation of a department and has a modernizing influence on other areas.

4.2 With financial support from DST, 4 *advanced interlinked multi-role centres* of research covering the eastern, western, northern and southern zones should be established. These may be set up in the following institutions where the necessary nucleus and infrastructure already exist: IACS (Calcutta), IIT Bombay, IIT Kanpur or University of Delhi, IIT Madras or IISc (Bangalore). Each of these centres should be provided with a minicomputer, with both number crunching and graphics capabilities, purchased from abroad (a typical example is VAX 11/780). Minicomputers are currently revolutionising large-scale computations. The initial investment for each centre may be only about 30 lakh rupees, followed by 5–10 lakh rupees every year. Centre personnel may consist of chemists, physicists, mathematicians and computer scientists. Future interlinking, through satellite, to a national computer grid may also be envisaged.

Each centre should undertake, in a concerted way, the following jobs: (a) *Research*, (b) *Teaching* (of advanced courses), (c) *Organization/Interaction*, and (d) *Service*. By turn, it should organize (i) Winter/Summer schools for teachers, (ii) Winter/Summer schools and workshops for research workers; (iii) Informal get-togethers, in the spirit of e.g., the Gordon Conferences. It should also develop a program bank, with essential programs in running condition. A university teacher or a research worker who has neither computing facilities nor his own program may visit the centre for a short period and get his calculations done. Each centre might concentrate on certain characteristic areas of strength. Thus, *these 4 centres would serve as beacons reassuring and quiding other Indian theoretical chemists. Together, they would be the prime movers for catapulting India into the international arena of the subject.*

4.3 An International Congress in Theoretical Chemistry should be organised in India once in every 4 years, by inviting the cream of international theoretical chemists. Each of the above 4 centres may organize this Congress, by turn.

4.4 Draw very bright and talented youngsters from chemistry, physics and mathematics (if possible). Nurture them by improving their *work conditions* and *financial benefits. This type of basic research requires people of originality, vision and courage*. The Indian society must learn to recognize the worth of the research scientist and take good care of him. *It is frightening that many of the finest young minds are forever lost from science* while the society happily offers lucre and prestige to the undeserving and the unproductive.

4.5 Institutions should attract talented young Indian Ph.D.'s from abroad and India on a contractual service for 5 years as Research Assistant Professor. During this period they may be given a free hand.

4.6 Explore and increase the interface with industry, e.g., through the design of new drugs, catalysts, conducting, semi- and superconducting materials, etc.

4.7 Funding agencies should strongly support any work in theoretical chemistry which leads to new concepts, new formalisms, new and viable large-scale computer programs. They should also provide equipment grants to individual research workers for purchasing desk-top microcomputers.

4.8 *Teaching*

4.8.1 Introduce *computer programming* at the B.Sc. level.

4.8.2 Introduce one or two *mathematics* courses for M.Sc. students in chemistry.

4.8.3 For M.Sc. students in physics and chemistry, teach *atomic and molecular phenomena* as a rigorous interdisciplinary subject and teach a course on *statistical mechanics* of equilibrium and nonequilibrium phenomena. These may be followed by a course on molecular organization, macromolecular assembly and the *evolution of life.*

4.8.4 Leading research workers may visit, by turn, selected universities for one or two months and deliver an intensive series of lectures on a chosen subject.

4.8.5 UGC should initiate an exchange programme for teachers and research workers.

4.8.6 Prepare entertaining educational films or video cassettes on chemical binding, molecular spectra and molecular structure, molecular reaction dynamics, critical phenomena, molecular evolution, etc. for wide distribution.

4.8.7 Theoretical chemistry should be regarded as a 4th discipline in chemistry, in addition to inorganic, organic and physical chemistry.

5. ACKNOWLEDGEMENTS

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APPENDIX I

A Cross-Sectional Bibliography of Theoretical Chemistry Research Done in India*

A. *Quantum Chemistry (including Quantum Biology)*

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*1. 'P' denotes contribution from a Physics Department.
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B. *Statistical Mechanics*

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C. *Non-Equilibrium Thermodynamics*

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Appendix II

*Brief Questionnaire**

(1) What are the specific areas in theoretical chemistry in which our country has made an impact on the international scene, as evidenced by, e.g., citations in international scientific literature?
(2) What are the strongest areas in theoretical chemistry in our country where considerable work has been done, arranged in order of strength?
(3) What are the fifteen to twenty most significant emerging or frontier areas in theoretical chemistry in the international scene, arranged in order of importance?
(4) What are the ten strongest institutions in India in theoretical chemistry, arranged in order of strength?
(5) What concrete steps would you suggest to improve the teaching of theoretical chemistry at the undergraduate or M.Sc. level?
(6) What concrete steps would you suggest to give a strong spurt to theoretical chemistry research in our country?

Apart from this, we also seek your help in preparing the final status report on the subject. Again, we would be grateful if you would be kind enough to

* Sent to more than 50 Indian theoretical chemists. About half of them responded.

provide us a summary of the work done in India by your group in the period 1970–82. The write-up may include (a) research topics, (b) summary of work done in each topic, (c) publications, (d) new concepts and formalisms developed, (e) new indigeneous computer programs developed, (f) any other original work done.

NEWS

MUSHROOMS: PROTEIN FOR THE THIRD WORLD?

. . . "Protein deficiency is not restricted to persons living in the developing nations, but there the condition is often particularly acute. Anything that can add protein to the diet in such countries is desirable. . . . The mushroom produced from agricultural and industrial discards contain 30–50 % protein on a dry weight basis, and about 3–5 % on a fresh weight basis. This proportion is twice that of asparagus and cabbage, four times that of oranges and twelve times that of apples. Growing mushrooms for food protein requires less land than producing protein from animal and other plant sources, especially if the land used to produce raw materials for mushroom cultivation (*e.g.*) the straws of agricultural crops, cotton wastes from the textile industry, and horse manure) is not taken into consideration. . . . All mushroom proteins contain all nine aminoacids essential for man, they are especially rich in lysine and leucine which most cereal foods lack . . ." (Reproduced with permission from *Press Digest, Current Contents*® No. 38, September 17, 1984. Copy right by the Institute for Scientific Information®, Philadelphia, PA, USA).

ARE THE FRUITS OF RESEARCH AVAILABLE TO ALL?

. . . "There is considerable evidence in the psychological literature that perceived status of ten has a major effect on behavior. The primary purpose of the present study was to examine the effects of two status variables in an academic setting by monitoring reprint-sending behavior. Reprints were requested from 1,200 authors of psychological articles by men and women of varying academic rank. Neither sex nor academic rank of requester had any significant effect on the total number of responses returned. However, male requesters received responses significantly faster than did female requesters. In addition, subsequent analyses indicated that reprint requests were more likely to be honoured by male authors than by female authors." (Reproduced with permission from *Press Digest, Current Contents*®, Number 29, July 19, 1984. Copyright by the Institute for Scientific Information® Philadelphia, PA, USA.)