Narmada valley is thus far from being seismically quiet. The reported assurnce[18] of the concerned engineers that 'they will take all possible safety measures while designing the dam, so that it is not affected even if earthquakes of M6 occur' is not adequate, for at least one earthquake of magnitude 6.3 did occur in this region. While the non-availability of the concerned gravity map of the Koyna region prior to the construction of the koyna dam can possibly be accepted as an excuse for not consulting a gravity map, the same cannot be said in the case of the Narmada valley region for which reliable gravity maps are now freely available. Since precise prediction of earthquakes is not possible, about the best one can do is to so design the structures that they can withstand earthquakes of magnitude 6.5 if not 7.0.

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NEWS

Give theoretical chemistry a push, says meeting

In the second in the series of such meetings (the first was held at Panjab University, Chandigarh, in 1986) in theoretical chemistry sponsored by the Indian Academy of Sciences ('Trends in theoretical chemistry', Indian Institute of Technology, Madras, 30 September to 1 October 1990), thirty-five theoretical chemists discussed directions for future work and co-operation among theoretical chemists as well as experimentalists, physicists and mathematicians.

The first session on statistical mechanics of condensed phases opened with R. V. Gopala Rao (Jadavapur University, Calcutta) giving a review of statistical-mechanics studies of equilibrium and non-equilibrium properties of liquids and solutions. The general approach was to apply perturbation theory to a hard-sphere model of the potential of interaction to compute structure functions, which leads to excellent agreement with experiment. S. Yashonath (Indian Institute of Science, Bangalore) discussed the molecular-dynamics simulation of a set of 64 diatomic particles interacting through a Lennard–Jones potential. K. L. Sebastian (Cochin University) talked about the profile of diffusion of a single particle on the surface of a regular lattice. The method proposed by him involves a normal co-ordinate analysis in the harmonic approximation near the transition state to predict possible states.

Density functional theory, to which the second session was devoted, was rather poorly represented. S. K. Ghosh (Bhabha Atomic Research Centre, Bombay) sketched his development of a density-functional theory for time-dependent systems characterized by external scalar and vector potentials. He derived single-particle Kohn–Sham-like equations for the time-dependent situation for the direct calculation of charge density and current density.

The third session was devoted to molecular structure. A. B. Sannigrahi (IIT, Kharagpur) introduced his definition of multi-centre bond index derivable from the SCF density matrix. E. D. Jemmis (University of Hyderabad) showed how the diagonal relationship in the periodic table and the principle of isolobal analogy could be used to predict the existence of unusual structures of organosilicon and siloboranes. S. Ramasesha (IISc) presented his method of theoretically modelling organic ferromagnets. M. S. Gopinathan (IIT, Madras) presented his modified version of the multiple scattering X-alpha theory for molecules, which takes into account relativistic and correlation effects, and can be carried out on a PC even for large molecules.

The session on interface of theory and experiment dealt with theoretical work directly connected with interpretation of experimental results. Anil Saran (Tata Institute of Fundamental Research, Bombay) spoke on quantum-mechanical PCILO studies on the conformation of anti-AIDS agents. His results indicated remarkable similarities among the conformational profiles of various anti-AIDS agents. P. T. Manoharan (IIT, Madras) presented MS–Xα and EHT results for the geometry and electronic

transitions of the normal and metastable states of $Fe(CN)_5NO^{2-}$ ion. B. Viswanathan (IIT, Madras) described how his model EHT calculations on heteroply acids can be used to rationalize the Bronsted acidity in terms of the charge on the oxygen atom. S. Subramaniam (IIT, Madras) demonstrated that *ab initio* calculations at the minimal basis set level can give very satisfactory results for magnetic susceptibilities for molecules. P. C. Mishra (Banaras Hindu University) presented both experimental results as well as quantum-mechanical calculations to prove that guanine can exist in two stable tautomeric forms, one of them corresponding to the form in DNA and only one being able to complex with oxygen. These results have possible connection with carcinogenesis and photodynamic action. P. C. Deshmukh (IIT, Madras) discussed the importance of electron-correlation effects in atomic photoabsorption processes, with special emphasis on autoionization resonances. S. R. Gadre (University of Poona) gave a semi-popular evening lecture on bounds and parallel computing. He explained the great advantages of parallelization of programs and the use of quantum-mechanical inequalities for speeding up *ab initio* computations.

The fifth session consisted of talks on molecular dynamics. B. L. Tembe (IIT, Bombay) described how the dynamics of solvation in model systems could be studied by molecular-dynamics simulation and how the relaxation times for time-dependent friction and for time-dependent cavity fields could be obtained. N. Sathyamurthy (IIT, Kanpur) summarized the methodology involved in time-dependent quantal approach to reactive scattering. He presented results for collinear $He + H_2^+ \rightarrow HeH^+ + H$, and showed that the information-theoretic entropy in phase space rose to a maximum as the system evolved in time. B. Cherayil (IISc) presented his effective-Hamiltonian approach to computation of thermodynamic properties of polymer solutions, which exploits the similarities between polymer solutions and other molecular liquids. M. K. Mishra (IIT, Bombay) presented an update of his work on the role of potential structure in nonadiabatic collisions. S. Kumar (IIT, Kanpur) demonstrated the occurrence of fractals in atom–molecule collisions using rotationally inelastic HF–Li system as an example. A. K. Mishra (Central Electrochemical Research Institute, Karaikudi) discussed the use of many-body theory in computing binding energy and identifying the change of valence orbitals on adsorption.

Development of computational formalisms was the theme of the sixth session, which opened with P. K. Mukherjee (Indian Association for the cultivation of Science, Calcutta) discussing a time-dependent perturbation theory for calculating doubly excited autoionizing states. Results for He-like systems were presented. S. Pal (National Chemical Laboratory, Pune) discussed a variational-cluster method having the desirable features of size extensivity and satisfaction of Hellmann–Feynmann theorem. K. Bhattacharyya (University of Burdwan) presented a sequential approach to divergent perturbation expansion. S. P. Bhattacharyya (IACS) presented the method of simulated annealing in electronic-structure calculations, which involves a global-minimal search utilizing metropolis algorithm at a sequence of temperatures. N. Sukumar (Panjab University) argued that, using field-theoretic ideas, the quantum theory of radiationless nonadiabatic processes can be reformulated in a manner analogous to that of radiative processes. D. D. Sarma (IISc) presented results of calculations on the electronic structure and metal–insulator phase diagram for CuO_2 square-planar lattice using a Hubbard model. S. N. Rai (North-Eastern Hill University, Shillong) outlined his calculations of reaction rates using quantum transition rate theory.

The last scientific session opened with a talk by V. Balakrishnan (IIT, Madras) on stochastic models of transport in disordered media. He presented results for first passage time properties for various types of random walks. P. K. Chattaraj (IIT, Kharagpur) described how hydrodynamic versions of several classical nonlinear-dynamical equations can be obtained and discussed the quantum equivalence of classical transition from toroidal motion to chaotic motion.

In a general discussion of the status of theoretical chemistry in India and its possible future directions, important points that emerged were:

1. Something should be done urgently to rectify the present situation in which theoretical chemistry is hardly taught and is not a subject of research in most state universities.
2. Statistical mechanics is also virtually ignored at the university level. This is unfortunate in view of its growing importance not only in chemistry, but in physics, engineering and biology.
3. A national computing facility that could be used by those who do not have easy access to such facilities is desirable. Some felt that distributed computing facilities would work better.
4. A program pool for sharing computer programs is desirable.
5. For the sake of greater academic and personal interaction among scientists in India, the setting-up of nation-wide computer networking facilities should be encouraged.
6. Parallel computing and the use of transputers are to be encouraged. However, many scientists expressed their unhappiness over some agency like C-DAC (Centre for Development of Advanced Computing, Pune) attempting to monopolize the production and distribution of hardware for parallel processing. They deplored C-DAC's recent action of initially promising hardware support to many scientists in India and inviting scientific proposals from them that utilize parallelization but finally backing out and asking the scientists to approach other funding agencies to support C-DAC activities. The scientists strongly felt that free-market forces should be allowed to operate in the production and sale of transputers/parallel cards.
7. On the educational front, theoretical chemists should make a special effort to write modern syllabi and textbooks for the use of school and university students and teachers. Efforts should also be made to conduct more workshops aimed at university students and teachers and the lecture notes of these workshops should be published for wider use by students and teachers.

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