

Many-electron theory*

A conference on the advances in many-electron theory was held recently. The meeting was attended by renowned experts in the field, including 40 senior faculty from India and abroad, and about 25 students from India. Several topics concerning many-body structure with emphasis on multi-reference theories and inclusion of relativistic effects, dynamics with special emphasis on non-adiabatic effects as well on density functional theory and some applications of the theory were covered during the conference.

A major focus of the conference was on the treatment of electron correlation effects in many-electron theory. In fact, the conference opened with the talk by Jean-Paul Malrieu, who has contributed enormously in the field for several years, on reference-independent excitation amplitudes in multi-reference methods resulting in new algorithms based on multi-reference second-order perturbation and coupled-cluster methods. Most multi-reference state-specific methods start with an expression of the wave operator with amplitudes being reference-dependent. This talk suggested a strategy to describe reference-independent amplitudes. The speakers and discussion leaders/chairs in this field included, apart from Malrieu, leaders like Debashis Mukherjee, Hans-Joachim Werner, Seichiro Ten-no, Henryk Witek, Wenjian Liu, Leszek Meissner, Trond Saue, Jozef Noga, Piotr Piecuch, Lucas Visscher, Masahiro Ehara, Jacek Korchowiec, B. K. Sahoo, M. Durga Prasad, Sourav Pal and a few young practitioners from India. The talks and discussions were centred on methods and algorithms based on multi-reference theories, understanding of static and dynamic correlation, vibrational coupled-cluster method, developments in equation-of-motion cou-

pled-cluster (EOMCC) method, inclusion of complex absorbing potential on powerful bound-state methods of EOMCC, symmetry adapted configuration interaction to describe resonant and decay states, inclusion of relativistic effects in EOMCC-based methods and others, treatment of explicit correlation using functions containing r_{12} terms within coupled-cluster methods, an extensive method to obtain an analytic treatment of helium atom wave function, etc. From the various topics covered, the emphasis was on improving or inclusion of important effects in coupled cluster (CC) and related methods. CC-based methods, in general, are established for reliable description of dynamic correlation and yet there are many important effects, described above, which need to be included or described with CC methods to make the theories more appropriate for a wider range of problems. Discussions were centred particularly on strong correlation effects and inclusion of static correlation and it was gratifying to note that early work in this area emerged from the group of Debashis Mukherjee in India and that in general, work done from India is in the frontiers.

A second general area covered in the conference concerned quantum dynamics, in particular, inclusion of non-adiabatic effects. Speakers and discussion leaders in this area included Todd Martinez, K. R. Shamasundar, A. J. C. Varandas, N. Sathyamurthy, and Satrajit Adhikari, among others. Several formulations of non-adiabatic dynamics for ground and excited states, their fast implementations in computers, consequences in terms of geometric phases, and development of accurate potentials for carrying out dynamics were discussed in the meeting. The discussions were at the frontiers of current research.

In addition to the above two major areas covered, there were talks in the area of density functional theory. There were interesting discussions based on the role of Hohenberg–Kohn theorem in density functional theory. Talks were also delivered on time-dependent density functional theory and quantum fluid dynamics approaches and multi-reference

density functional theory. Treatment of static and dynamic correlation was realized to be important in the description of multi-reference density functional theory. Speakers in this theme included Trygve Helgaker, Swapan Ghosh and Andreas Savin.

During the conference there were also discussions on interesting applications using different *ab initio* and density functional theories highlighting the effects of electron correlation. Some of the themes addressed were on holes in borophene systems, noble gas binding ability of boron clusters, quantum phase transitions in low-dimensional optical lattices, π -distortivity problem, symmetry breaking in low-dimensional flat materials, catalytic electron in photochemical bond dissociation cooperativity effects in non-covalent interactions, *ab initio* calculations in prediction of molecular magnets, electron transfer in complex environments and electric field effects in molecular clusters. E. D. Jemmis, Pratim Chattaraj, Swapan Pati, K. L. Sebastian, Ayan Datta, Ankan Paul, G. Narahari Sastry, G. Rajaraman, Debashree Ghosh, G. Naresh Patwari, Sandip Kar and Rajarshi Chakrabarti spoke on the origin of mixed population during neural stem cell development and the dynamics of nucleic acids in the presence of carbon nanostructures respectively.

In addition to the invited talks, there were posters presented by about 24 students which highlighted the role of theory and computational chemistry in the solution of problems in chemistry and materials. Posters focused on many topics of current interest, namely on hydrogen activation, cross-coupling reactions, hydrogenation of carbonyl compounds as well as carbon dioxide, transition metal-free C–C bond activation, modelling surfactant interactions, CO release from organic molecules, application of non-adiabatic dynamics to different systems, quantum rotor orbital excitation originating from dynamic Jahn–Teller effects, evolutionary algorithm in configuration interaction, relativistic EOMCC, biological applications using quantum mechanics/molecular mechanics approach, etc.

*A report on the conference on ‘Recent Advances in Many-Electron Theory – 2017’ (RAMET-2017) held in Goa, and jointly organized by the Indian Association for the Cultivation of Science, Kolkata and Indian Institute of Technology Bombay, between 9 and 12 February 2017. The conference was convened by Sourav Pal (IIT Bombay), Satrajit Adhikari and G. P. Das (IACS, Kolkata).

The conference laid particular emphasis on developments of multi-reference-based electronic structure formulations and dynamics with special emphasis on non-adiabatic quantum effects. It was heartening to note that the Indian contributions in the above areas were well recognized in the conference. The pioneering contributions of multi-reference developments, in the context of coupled cluster theory, were highlighted by several speakers. In fact, much of the work

in this area has been generated from the ideas that originated in India. The contributions from India on the recent developments of complex absorbing potential-based CC theory as well as relativistic equation of motion CC theories were also acknowledged by talks in these areas. The work of Indian groups on dynamics, in particular, non-adiabatic quantum dynamics, also attracted attention. The conference also noted strengths of India in the area of density functional

theory and it was clear that some good applications of the theory have emerged from our country.

This conference brought out the strength of theoretical chemistry, in particular quantum chemistry, in India.

Sourav Pal, Department of Chemistry, Indian Institute of Technology Bombay, Powai, Mumbai 400 076, India.
e-mail: spal@chem.iitb.ac.in

MEETING REPORT

National Conference on Technology Vision*

At the National Conference on Technology Vision 2035, the visions for four sectoral areas – health care, Information and Communication Technologies (ICT), education, and safe and speedy mobility were discussed and reviewed. It was attended by educators, health professionals and students from schools and colleges in Hyderabad.

The inaugural session was presided over by Anil Kakodkar (TIFAC, National Apex Committee and Technology Vision 2035). Y. S. Chowdary (Minister of State for Science and Technology & Earth Sciences, Government of India) released the Medical Sciences and Health Care Technology roadmap document. W. Selvamurthy (Technology Vision 2035 Medical Sciences & Health Care sector) and Gautam Goswami (Technology Vision 2035) also participated in the inaugural session. The session emphasized on the significance of the vision by characterizing technology as the bedrock on which comprehensive national power could be built to empower the citizens, societies, nations and strategic autonomy of the nation. It was observed that R&D investment in India needs to be more productive and industry-driven. An integrated approach should be developed

inculcating our traditional medicine, offering the motto ‘From a Document to a Movement’, hoping that young minds would take the vision in the document forward. Suggestions were given to TIFAC to take a closer look at neglected diseases, which are not lucrative for pharmaceutical firms develop treatments for them. It was desired to implement a 5-year rolling plan for Technology Vision 2035 as well as a monitoring mechanism by TIFAC.

The first plenary session on the first day on universal healthcare and public hygiene was chaired by A. P. Jayaraman (Trustee, IDF) and B. Narayan Iyer (CEO, IDF) and attended by Nirupam Madaan (AIIMS, New Delhi), K. V. S. Prasad (Sanzyme) and D. T. Selvam (Defence Research & Development Establishment (DRDE), Gwalior). The discussion noted that India was ranked 143rd in the Sustainable Development Goals index. It identified the following core issues: (i) lack of vision and direction; (ii) inadequate financial resources; (iii) a skewed distribution of resources and (iv) any new model has to gain cultural acceptability, be accessible, comply with legal framework, and also be a viable business model. The discussion exhorted that a culture of cleanliness was urgent, with special attention to kitchens and hospitals to improve public hygiene. Further discussion focused on the importance of public health, threats of biological and chemical warfare, developing near-future technologies such as bacterial

identification without using body fluids, susceptibility status of pathogens without culture and multivalent vaccines for immunizing against multiple pathogens.

The second plenary session was on maternal and child health. Sangeeta Gupta (ESI Post Graduate Institute of Medical Science and Research, New Delhi), A. T. Dabke (Chhattisgarh Ayush and Health Science University, Raipur); Mahita Reddy (Government Maternity Hospital, Hyderabad) and Swathi Aarya (PG OB-GYN) led the discussions. The speakers informed the audience that: (i) most maternal deaths were still from preventable causes such as haemorrhage and sepsis; (ii) one in three malnourished children is Indian, and (iii) a low-BMI mother is prone to deliver a low-birth weight baby which is more susceptible to health problems such as hypertension, diabetes and obesity. While discussing the schemes in effect at present like the Dakshata programme for nurses and doctors, they emphasized the need to provide high-quality childbirth services at PHCs, and expressed hope in best technological practices from around the world, including mobile apps for data collection and communication (such as Umeed Say in Pakistan). Anaemia was also discussed in depth, including the causes besides just iron deficiency. Prevalence of anaemia in 65–75% people in India compared to 51% in other developing countries was found to be especially worrisome. Measures to improve the situation included ensuring food fortification with iron-rich

*A report on the National Conference on Technology Vision 2035 held on 29 and 30 September 2016. The conference was organized by the Indian Development Foundation at the Oakridge International School, Hyderabad along with TIFAC.