

## Research expedition of Prof. Eluvathingal D. Jemmis

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Professor Eluvathingal D. Jemmis, completed 60 years on 31 October 2011. For the past 40 years, he dedicated his life to fundamental chemical research in India. His pioneering research career resulted in the publication of around 200 original research articles (about 40 of them in JACS). Professor Jemmis silently but most effectively transformed the way in which experimentalists perceive theoreticians in India. He has trained more than 25 Ph.D. students, and several of them have emerged as leading computational chemists, biologists, and material scientists. His accomplishments in research have resulted in several awards and he is elected as a fellow of all the three science academies of India, and also of the academy of sciences for the developing world.

In retrospect, it was probably a very tough call—to move from the most modern research University in USA to a budding university in India. The dream was big—to make *pioneering efforts* in applied theoretical chemistry, to

*carryout excellent research* in computer-aided methods of chemical analysis, *to introduce a new topic* of chemical research (computational chemistry) in the nation, *to establish* new concepts in molecular orbital theory, *to design* new molecules with novel material properties on the one hand and biochemicals with drug-like properties on the other, and *to educate* the next generation of leaders in computational chemistry. The facilities were none—not a single computer on the university campus, only one computer in a nearby city (~40 km away). At the social level, the move was from one of the most modern campus of the world with all facilities to a campus of a nascent university with no facilities (a land filled with bushes and stones, with absolutely no communication facilities); the only thing known was that the administration of the new place had progressive plans. This was the background in which Professor Jemmis decided to move to University of Hyderabad in 1980 after receiving research training in premier institutes such as IIT (Kanpur), Princeton, Erlangen, and Cornell Universities.

The journey starting from Ithaca, USA, indeed turned out to be more rewarding than the journey to 'Ithaka' as described by Constantine Cavafy. After 30 years of enduring efforts, Prof. Jemmis became a pioneer in computational chemistry to be well known across the world. He made strong efforts to give greater importance to C in QC (Quantum Chemistry) and won the admiration and accolades from experimentalists. His contributions in molecular orbital theory helped in establishing the concept of overlap control and stability of polyhedral molecules; contributions in organometallics provided important clues to numerous catalytic processes; contributions using electronic structure methods led to the identification of analogy between divalent silicon and trivalent boron; contributions in cluster chemistry helped in introducing the mno rules (also known

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as *Jemmis rules*) and led to a relationship between polyhedral boranes and allotropes of elemental boron similar to the structural connection of benzene to graphene; contributions in material science helped in generating novel boron clusters; contributions in nano science resulted in the concept of boron buckyball; contributions in biomedical sciences helped in designing novel lead compounds for anti-asthmatic effects and anti-tumor effect; collaborative efforts helped in developing synthetic strategies for the generation of many new organic molecules.

In addition to the above research contributions, Prof. Jemmis is also involved in institution building and thus

nation building. His efforts in teaching helped in creating several leaders in computational material science and computational drug discovery. Prof. Jemmis was instrumental in the establishment of Centre for Modeling, Simulation and Design (CMSD at University of Hyderabad), and enhancement of computational facilities at SERC (at Indian Institute of Science, Bangalore). He is currently busy in the establishment a new institute for research and teaching in basic sciences (IISER, Thiruvananthapuram).

It is with a great sense of gratitude, we present this festschrift in honor of Prof. Eluvathingal D. Jemmis on this day.