

## Preface

This Special Issue of the Journal of Chemical Sciences is brought out to honour Professor Charusita Chakravarty who passed away on 29<sup>th</sup> March 2016, after a prolonged battle with cancer. She is survived by her husband and her daughter, and a large number of students and colleagues who were inspired by her brilliance, honesty and commitment to an academic life that meant a lot to her. Any death is sad but in Charu's case, this untimely death cut down a blossoming scientific career that was having a positive impact on the Indian scene of the kind not seen before. It is indeed difficult to believe and accept. As one can see from the large number of quality contributions contained in this Special Issue, the respect and admiration is widespread.

Born in Cambridge, Massachusetts, USA on 5 May 1964 as the only daughter of the economists Sukhamoy and Lalita Chakravarty, Charu grew up in a liberal academic environment in Delhi. She chose to give up her American citizenship and become an Indian citizen when she was in her twenties. Charu was brilliant in her studies and this was reflected in her topping the Delhi Higher Secondary Board. She was selected as a National Science Talent Scholar and also cleared the highly competitive Joint Entrance Examination (JEE) of the IITs in 1982 (in those days there was no coaching!). She wanted to join the five-year integrated M Sc programme in chemistry in IIT Kanpur, even though her JEE rank made her eligible to join the B Tech programme in one of the engineering disciplines. However, at the suggestion of a family friend and that of her father she joined B Sc (Hons.) in Chemistry in St. Stephen's College, Delhi. After graduating from Delhi University with a gold medal in 1985, she joined Cambridge University, UK, to do the Natural Sciences Tripos, obtaining First Class Honours in Natural Sciences, Part II Chemistry in 1987.

Charusita studied for a PhD under the supervision of Professor Sir David Clary at Cambridge University during 1987–1990 (DC is one of the Guest Editors of this Issue). She joined Professor Clary after taking his course in molecular scattering theory in her third undergraduate year and this introduced her to this field of research.

Even though Professor Clary was away on sabbatical in the USA for the first six months of her PhD course, she still wanted to join Professor Clary's research group. As a result, she started her research almost independently at Cambridge in October 1987. Her first project was on the theoretical aspects of the dissociation kinetics and dynamics of molecular ions. She wrote a fine paper on this subject which, according to Professor Clary, was essentially all her own work. This was a very mature achievement for a first year PhD student.

In a testimony to Charusita Chakravarty's later (and also early) science development, Charu wanted a research topic which was more closely linked to recent experimental work. Professor Clary thus recommended Charu to work on new measurements of the spectra of the van der Waals complex ArOH that were being performed by Professor Marsha Lester from the University of Pennsylvania. Charu was at once enthusiastic and this started a very productive collaboration with Professor Lester's group. She wrote her own computer codes to calculate the spectra and predissociation parameters of ArOH from first principles. This led to one of the best characterised weakly-bound complexes, in both the ground and electronically excited states, where *ab initio* theory and experiment agreed almost perfectly. She wrote an excellent PhD thesis which was examined by Professor Jeremy Hutson FRS. Six papers came out of this research and they have been quite highly cited.

Charu then went to do postdoctoral research at the University of Santa Barbara working with Horia Metiu on theoretical surface science. She learned a lot which she found of great use in her future research. She continued research in New Delhi for a short period and then won a highly prestigious Gulbenkian Junior Research Fellowship at Churchill College, Cambridge. This allowed her to initiate her own independent research programme on the path integral simulation of clusters and condensed phases which she continued for the rest of her career. This research also set her up well for the tenure-track post she then took up in the Indian Institute of Technology Delhi.

We should mention two important contributions that Charu made completely independently in the later part of her career. One is the establishment of an elegant relationship between the diffusion of a molecule and the entropy of the liquid for water-like molecules. Many Indian theoretical chemists followed up on this work. This drew great deal of international attention. She also made a notable contribution to the universality (or, rather the lack of) of Lindemann criteria of melting of solids.

It is still hard to believe that Charu has died at the young age of 51 at the peak of her research

career. In the last year of her life even when she was very ill she found working with her students quite therapeutic. The many excellent papers she wrote serve as a permanent testament to her dedication to science.

Indian, indeed international, science, and theoretical physical chemistry in particular, suffered a great loss in Charu's death. Through this Special Issue we hope to remember not only her contributions but also her commitment to science and the diversity of the problems studied.

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