comments and feedback. This was evident in a recent discovery of arsenic-utilizing bacteria, published in *Science*.

Richa Malhotra (S. Ramaseshan Fellow, *Current Science*) spoke on the issues of science journalism in the print medium and possible ways to overcome them. These were based on her interactions with well-known science journalists from India. To overcome the issue of credibility of science in newspapers, Malhotra suggested that agencies could employ a 'fact-checker' (a science graduate) to check if all the stories on science are factually correct. Suchitra Mathur (IIT-Kanpur) traced how science fiction could be used as a medium to communicate science and explored a host of issues related to the teaching of science in India. She expressed concern over the fact that the Indian system of education does not expose science students to science as a discourse – that history of science is never told.

Sarah Davidson (Cornell University), and H. N. Chanakya (IISc), presented case studies of interacting with villagers, the involvement of farmers and local knowledge. Davidson focused on how genetically modified papaya got into debate in Thailand. Deepak Kumar (Jawaharlal Nehru University, New Delhi), in his keynote, presented a historical perspective of science, where he anecdotally described how science changed from pre-colonial to colonial science. S. Ranganathan (National Institute of Advanced Studies, Bangalore) being a scientist mentioned his role as a communicator in disguise.

Best discussions usually happen over a cup of coffee. This was noticeable in the World Café at the workshop conducted by N. S. Anuradha (IISc). Participants shared and discussed ideas to enhance science communication and learn about science in multicultural societies, and ways to embrace multiple perspectives. The discussion brought to light that there are clear divides relating to rural–urban, gender, language and access to technology when it comes to communication. Thus, remote areas should be studied for what they need in terms of information from science and then communicated with, rather than communicating and later learning what was needed. Use of technologies such as mobile phones and video conferencing needs to be further exploited. To make the interaction two-way, one strategy could be forming a group of semi-experts that could act as mediators between scientists and laymen.

The IUSSTF was established in 2000 with an aim to promote, catalyse and seed 'bilateral collaboration in science, technology, engineering and biomedical research through substantive interaction amongst government, academia and industry' (http://www.indousstf.org/). The activities of the forum include fostering exchange programmes, visiting professorships, travel grants, research fellowship awards, training schools, workshops, conferences, symposia, etc. Some of its popular programmes are Standford–India Biodesign Fellowships, Khorana Program for scholars, visiting fellowships in nanotechnology and innovation growth program. Another internship opportunity recently instituted is the Viterbi–India Program.

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MEETING REPORT

Molecular interactions*

Although a bond between two atoms in a molecule is fairly well-understood, intermolecular interactions remain at the heart of chemistry and biology. Hydrogen bonding is the most important of intermolecular interactions, as it controls the properties of the molecules of life, water and DNA. While the importance of these strong O–H···O and N–H···N hydrogen bonds in life has been well-recognized for long, some recent studies reveal that weak hydrogen bonds may play a crucial role in anesthesia. Advances in various experimental and theoretical techniques are contributing to shaping and enhancing our understanding of all these molecular interactions. A discussion meeting on 'molecular interactions' was organized with the support of the Indian Academy of Sciences, Bangalore. The meeting attracted scientists working in diverse fields.

The meeting started with a brief introduction by E. Arunan (Indian Institute of Science (IISc), Bangalore), convener of the meeting. He pointed out that there have been several key advances over the last decade that challenged the conventional wisdom about hydrogen bonding. The stunning difference between the crystal structure close to the freezing point at ambient conditions, for ice (H_2O) at 0°C and H_2S at –60°C has led to the common perception of 'hydrogen bonding' and 'van der Waals interaction' as two distinguishable physical forces among chemists. The advent of molecular beam spectroscopy and scattering studies have showed that $(H_2O)_2$ and $(H_2S)_2$ have similar structures. Moreover, molecular beam electric resonance spectroscopy showed that the complex formed between HF and ClF had a structure HF···ClF, rather than the expected hydrogen bonded ClF···HF. Though it was originally called 'anti-hydrogen bond', it is now well-recognized as a halogen-bonded complex. The International Union of Pure and Applied Chemistry (IUPAC) recognized the importance of these phenomena and formed task groups to summarize our understanding of these phenomena and define hydrogen bonding and halogen bonding.

The meeting had 16 invited lectures and there were discussions during and after the talks. The topics ranged from the interaction between two rare gas atoms such as argon and neon to the interaction between the domains in multi-domain and multifunctional proteins. The first

*A report on the Discussion Meeting on Molecular Interactions held at Orange County, Coorg, during 28 November–1 December 2010.

talk was given by Tapas Chakraborty (Indian Association for the Cultivation of Science, Kolkata). He presented experimental results on some diketones in the gas phase, liquid phase and in a rare-gas matrix. Although keto-enol tautomerism is well known in chemistry, he pointed out that γ-cyclohexanedione existed only in the keto form in the matrix and formed dimers exhibiting C–H···O hydrogen bonds. Ashoka Samuelson (IISc, Bangalore) spoke about weak interactions in drug design and asymmetric catalysis. He presented some experimental results which suggested that $\pi\cdots\pi$ interactions occurring far away from a chiral centre could still influence enantio-selectivity. He suspected that such interactions having $\pi\cdots\pi$ distance of even 4–5 Å could be influential. This raised some discussions among participants about what would be the maximum distance between two π centres up to which they could have attractive interactions that are still influential. The first session ended with a talk by Ayan Datta (Indian Institute of Science Education and Research, Thiruvananthapuram). He spoke about understanding intermolecular interactions in complex systems through computations. Magnetic interactions through multi-centred π-stacked molecules and the interaction of one water molecule in calixarene (water in the smallest cup) were mentioned by him.

Judith Howard (University of Durham, UK) spoke in the second session and compared neutron and X-ray diffraction techniques to study molecular interactions. She pointed out that neutron diffraction is useful for locating H atoms but X-ray diffraction can give electron density topology in the crystal which is crucial in understanding bonding. C. Pulla Rao (Indian Institute of Technology, Mumbai) spoke on manifestations of weak interactions in complex molecules. He discussed lectin–carbohydrate interaction and also $Hg^{2+}\cdots\pi$ interaction which results in fluorescence enhancement in anthracenyl-glyco derivatives.

Pierangelo Metrangolo (Politecnico de Milano, Italy) spoke about halogen versus hydrogen bonding in crystal engineering. He showed that Br^- as acceptor could interact with partially positive Cl/Br/I in molecular complexes which are now described as halogen bonding but not F. After the talk, T. N. Guru Row (IISc, Bangalore) mentioned that his group has looked at cases where the electron cloud in F could be distorted leading to a 'halogen bond' with F as the positive end. G. Mugesh (IISc, Bangalore) discussed the role of intermolecular interactions in the synthesis and recognition of thyroid harmones. He emphasized the role of $^{\delta-}Se\cdots{}^{\delta+}I$ and $^{\delta+}Se\cdots{}^{\delta-}N$ interactions in these systems and showed their importance in the treatment of hyperthyroidism. Arunan spoke about hydrogen, halogen and lithium bonding and presented microwave spectroscopic results on unusual complexes formed between benzene and ethylene, and methane and hydrogen sulphide. He also cautioned against the blind extension of the hydrogen bond definition proposed by the IUPAC task group chaired by him for defining the halogen bond. He particularly showed that X–F stretching frequency in Y···X–F halogen bond is not a useful criterion for halogen bond as opposed to the H–F stretching frequency in Y···H–F.

Mrinalini Puranik (National Center for Biological Sciences, Bangalore) spoke about aromatic amino acids and substrates as probes of local environment and dynamics in proteins. She highlighted the importance of dynamics in addition to the steady state structures in determining the protein functions and how simulation of Raman intensities can help in these studies. Guru Row demystified the 'pharmaceutical cocrystals' and showed that there is no difference between cocrystals and salts. He also presented the crystal structure of adenine without water, characterized for the first time. He also summarized the extensive work his group has carried out on 'halogen bonding'. G. Krishnamoorthy (Tata Institute for Fundamental Research (TIFR), Mumbai) talked about site-specific dynamics in an RNA thermometer. He showed that a single mismatch in base pairing can lead to significant differences in the fluorescence anisotropy lifetime.

David Capelletti (Universita di Perugia, Italy) described how one can get intermolecular potentials from crossed beam experiments. Coupled with the state-of-the-art theoretical methods, he showed that charge transfer plays an important role in weakly hydrogen-bonded complexes formed between rare gas and H_2O and also H_2 and H_2O. Sanjay Wategaonkar (TIFR, Mumbai) discussed experimental results obtained from his molecular beam laboratory using spectroscopic techniques. Through a comprehensive study he showed that sulphur atom can be as good an acceptor for hydrogen bonds as are F, O and N. He also showed that in many of these 'hydrogen bonded systems' dispersion plays a crucial role.

Joanna Sadlej (University of Warsaw, Poland) showed how vibrational circular dichroism (VCD) spectroscopy can be useful in probing chirality transfer in molecular interactions. As the VCD intensity depends both on the electric and magnetic dipoles, particularly on the angle between them, it offers a unique tool for studying intermolecular interactions. Hanudatta Atreya (IISc, Bangalore) convinced the participants about the importance of Nuclear Magnetic Resonance (NMR) in elucidating inter-domain interactions in proteins. He presented results from both NMR spectroscopy and molecular dynamics simulation. V. Subramanian (Central Leather Research Institute, Chennai) made the last presentation for the meeting. He discussed the interaction between peptides and carbon nanotubes studied by classical dynamics simulation. He presented new results on adamentane–benzene interaction.

On the evening of 29 November 2010, there was a session dedicated to discussing the IUPAC provisional recommendation on the definition of the hydrogen bond, which is available at http://media.iupac.org/reports/provisional/abstracts/arunan310311.html. Arunan presented the recommendation to the participants. This was followed by stimulating discussion that lasted 90 min against the planned duration of 45 min. Several aspects of the definition were discussed in detail and Metrangelo observed that this would be useful to the task group set out to define the halogen bond.

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