

## GRC 2010 on crystal engineering – a crystallizing experience!\*

Neil E. Gordon, a chemist, initiated the Gordon Research Conferences (GRC) in 1931 at Johns Hopkins University. In the beginning, these meetings dealt with topics mostly related to chemistry. After the first few years, Gordon decided to move the conference to the better ambience of the New England area. These secluded areas, with least distractions, retained the participants for the entire meeting whereas cost-effective accommodations enabled wider participation of scholars and students from different countries. A free atmosphere to share unpublished results with an opportunity to receive immediate feedback are also some of the unique features of the GRC meetings. Further, the free afternoons are invaluable for socializing, relaxing and informal discussions. Overall, the format became quite attractive making GRC the Mecca of conferences. Over the years, the organizers started embracing frontier research areas in the biological, chemical and physical sciences, and their related technologies ([www.grc.org](http://www.grc.org)).

It is almost four decades since Gerhard Schmidt (Weizmann Institute) coined the term 'Crystal engineering' to describe the multidisciplinary subject of research for development of a fundamental understanding of intermolecular interactions to enable design of molecular solids with desirable structures and properties. It took a while to attract scientists to this emerging field initially, but it picked up speed in the last three decades. A need to organize a GRC on this rapidly emerging field was recognized by a small group of scientists led by Gautam R. Desiraju, who worked diligently to make it a reality at the Waterville Valley Resort. Desiraju, who is also the author of the first seminal monograph on this title and who has contributed in many ways to popularize this subject, was appropriately chosen to chair the first GRC. This event is widely recognized as a milestone and a new beginning (or the end of the beginning) for crystal engineering.

The conference was well represented by a broad spectrum of 160 participants

in this field coming from academia, industry and government laboratories from all parts of the world. Apparently, this had been one of the largest attendances on record for a first time GRC in any subject. A large contingent from India (made possible by the generous support of funding bodies like Department of Science and Technology, Council for Scientific and Industrial Research and Indian National Science Academy) may be another unique feature of the GRC. Whereas industry was well represented by American and European participation, it was also noteworthy for some active participation by the Indian industry. Global expansion of the pharmaceutical industry in India and their interest in solid materials is expected to further increase Indian industry participation at these conferences in the near future, and foster collaborations between scientists in academia and industry.

The general body meeting overwhelmingly voted to hold this conference at the same site in June 2012. As is customary in the GRC meetings, the vice-chair of the present meeting (Robin D. Rogers, University of Alabama) will be the chair of the 2012 meeting. The future sites for the conference also came up for discussion during these deliberations. Traditionally, GRCs are held at sites in New England, but the list of sites has been expanding to places in other parts of the US and Europe in recent years. We understand that a proposal to move some GRC meetings to a site in India has been mooted. Perhaps, it is the right time for the Indian scientific establishment to consider hosting of these meetings in India. This would be in keeping with the increased academic visibility of the Indian scientific community in the international arena. The conspicuous presence of a large number of Indians at this conference might also be helpful in gaining such a favourable reaction.

The conference featured several broad topics such as: (1) Design strategies for molecular organic solids, (2) Coordination polymers – structure, (3) Co-ordination polymers – function, (4) Polymorphism and crystal structure prediction, (5) Formation of crystals, (6) Process development and scale-up, (7) Organic reactions in the solid state, (8) Two-dimensional crystal engineering,

and (9) Future frontiers of crystal engineering. Each topic consisted of several invited talks by prominent scientists and was moderated by an expert discussion leader. Almost all the speakers laid emphasis on unpublished research from their labs and encouraged discussion of the future target areas. Discussion leaders (Christer Aakeroy, Örn Almarsson, Joel Bernstein, Neil R. Champness, Anthony W. Colemann, Len R. MacGillivray, Allan S. Myerson, Matthew J. Rosseinsky and Mike J. Zaworotko) utilized Q&A sessions to stimulate lively discussions on each of the topics.

The inaugural lecture was delivered by James D. Wuest (Canada) about the expanding scope of crystal engineering applicable to glass formation by systematic structure variation. Lourdes Infantes (Spain) discussed functional group competition and preferences in the formation of hydrates and multicomponent crystals. Stimulating lectures by Richard Robson (Australia), Shilun Qiu (China), Jeffrey R. Long (US), Christian Serre (France) and Susumu Kitagawa (Japan) opened up the world of coordination polymers with their potential applications in diverse areas from catalysis to medicine. Polymorphism is still an enigma to both pharmaceutical industries and academicians and a session devoted to this topic probed on how to map polymorphs on energy landscape diagrams. Colin Pulham (UK) highlighted high pressure techniques for exploring polymorphism in molecular materials, pressure induced crystallization and synergy with crystal structure prediction methods. Adam J. Matzger (US) underlined the importance of directional forces in inducing polymorphism. Sally L. Price (UK) briefed the strengths and weakness of computational strategies for calculating crystal energy landscapes. Peter Vekilov (US) and Roger J. Davey (UK) addressed the theoretical issues related to nucleation and the problems associated with the process of crystallization. In a session devoted to pharmaceuticals (process chemistry and scale up), Vincenzo Liotta (Merck), Magali Hickey (Alkermes), Matthew Peterson (Amgen) and Patrick Connelly (Vertex) shared their efforts and apprehensions in dealing with phase change (amorphous, polymorph or sol-

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vate/desolvate) that leads to drug degradation and loss of API (active pharmaceutical ingredient) during process development. The session devoted to reactivity in the solid state was quite illuminating. Jarugu N. Moorthy (India) addressed the effect of light in inducing, controlling and crystallizing new phases in the solid state by choosing appropriate organic solids; Gerd Kaupp (Germany) showed the significance of mechanochemistry and how reactions could be monitored with state-of-art-techniques. Two-dimensional crystal engineering is not only topical but assumes significant relevance to shaping industrial materials. Steven De Feyter (Belgium) and Paolo Samori (France) showed the significance of surface in influencing interfacial growth. Krzysztof Wozniak (Poland) and Katharina Fromm (Germany) contributed short presentations on electron density studies and silver coordination polymers respectively. The concluding session provided some thought-provoking projections about the future of crystal engineering by Marcus Neumann, Janet Scott, Mike J. Zaworotko and Peter Erk in their own inimitable styles. They touched upon some important issues related to the

challenging task of blind tests, applicability and limitations of crystal structure prediction towards realizing a virtual diffractometer and recognizing the signature of supramolecular building blocks in designing materials.

According to the GRC tradition and to allow all attendees to present their recent results, two poster sessions were organized. Senior researchers as well as graduate students participated in these sessions enthusiastically and presented a total of 110 posters on various topics of crystal engineering. These sessions facilitated a more detailed discussion of the results from various research laboratories. In addition to these formal interactions, the conference also provided a setting and ample time to allow informal discussions fostering new collaborations and joint efforts in the field. By all measures, the first GRC on crystal engineering was a big success and is poised to continue in the same trajectory into the future. On the scientific level, the conference highlighted the shortcomings of our capabilities to predict structure and function of solids based on the current understanding of inter- and intramolecular interactions, and the need for

better understanding of thermodynamics and kinetics of crystallization process. On the other hand, there were several successes that showcased design of desirable structures of metal organic frameworks with potential applications in storage and delivery of hydrogen and other materials, the potential benefits of co-crystals in formulating APIs, and durable implants coated with anti-infective drugs, etc. The current high level interest of Indian scientists in the field of crystal engineering and the significant impact they have already made in advancing this field are well positioned to contribute towards discoveries of solid materials useful in harnessing newer sources of energy, tackling problems of environmental degradation, and development of new implants and novel pharmaceuticals for better health of the growing world population.

**A. Ramanan\***, Department of Chemistry, Indian Institute of Technology Delhi, Hauz Khas, New Delhi 110 016, India and **Bhiseti Govinda Rao**, Vertex Pharmaceuticals, 130 Waverly Street, Cambridge, MA 02139, USA.

\*e-mail: aramanan@chemistry.iitd.ac.in

## MEETING REPORT

### Plant biotechnology: from basic research to crop improvement\*

In the coming decades, there is an urgent need to dramatically increase the world's food output whilst at the same time protect our environment. This will require a concerted effort among plant biotechnologists to improve plant traits, which will eventually result in higher productivity under resource-limiting or stressful conditions. An annual scientific meeting highlighted recent research activities within plant biotechnology. The conference was attended by more than 200 academic and industrial delegates and included scientific presentations from three keynote speakers and 22 talks from plant scientists around the globe. The meeting was organized into seven sessions: (1) Products and productivity, (2) Nutrition and diseases, (3) Breeding and systems biology, (4) Technologies,

(5) Public-private partnership, (6) Systems biology – a developer's tool and (7) Green growth. The meeting covered a wide range of plant biotechnology related topics such as medicinal importance of plant products, molecular adaptive strategies of plants, novel technologies to create, identify and utilize DNA sequence polymorphisms in crop improvement, next generation sequencing techniques and the role of biotechnology in eco-farming/organic farming and biofuel production. The meeting started with a welcome address by the head of the steering committee for PBD, Preben Bach Holm (Aarhus University, Denmark). He stated the importance of basic and applied plant research in the current era given the fact that plants form an integral part of our food, feed and fuel supply. The first keynote speaker in the scientific session, Rainer Hedrich (Institute for Molecular Plant Physiology and Biophysics, University of Würzburg, Germany) discussed the molecular aspects of stomatal closure in plants in

response to drought and the phytohormone abscisic acid (ABA). He presented experimental evidence that under drought conditions, ABA triggers stomatal closure by the release of anions from guard cells. His group has identified one of the novel guard cell anion channels in plants, SLAC1. In his talk, he presented evidence that SLAC1 is a key member of the signalling pathway leading to stomatal closure under drought conditions, and SLAC1 invariably requires a protein kinase OST1 and a phosphatase ABI1 to exert its function. SLAC1 seems to be a potential candidate gene involved in drought tolerance in plants. In an oral presentation during the same session, Michael D. Mikkelsen (University of Copenhagen, Denmark) highlighted the importance and effect of plant derived, cancer-preventing compound glucoraphanin on human health. Glucoraphanin is a cancer preventing compound derived from methionine in cruciferous plants. Essentially, its production involves 14 intermediates and 13 enzymes. By ex-

\*A report on the Annual Scientific Meeting organized by the Plant Biotech Denmark (PBD) (<http://www.plant-biotech.dk/>) during 4–5 March 2010 at LIFE, University of Copenhagen, Denmark.