Angewandte Author Profile

Angewandte International Edition Chemie

G. R. Desiraju

Gautam R. Desiraju

Date of birth:	August 21, 1952
Position:	Professor, Indian Institute of Science, Bangalore
E-mail:	desiraju@sscu.iisc.ernet.in
Homepage:	http://sscu.iisc.ernet.in/gautam_r_desiraju.html
Education:	1969–1972 BSc, St. Xavier's College, University of Bombay 1972–1976 PhD supervised by David Y. Curtin and Iain C. Paul, University of Illinois, Urbana
Awards:	**2000** Humboldt Forschungspreis; TWAS Award in Chemistry; **2011–2014** President, International Union of Crystallography
Current research interests:	Crystal engineering is the designed synthesis of functional molecular solids. In our research group, we handle many aspects of this interdisciplinary subject, ranging from synthetic methodologies with supramolecular synthons, to the study of intermolecular interactions and their characteristics, polymorphism, pharmaceuticals, and computational and experimental studies of the crystal-structure landscape. We use cryocrystallography, charge density analysis, and crystal-structure prediction to understand and design new crystal structures.
Hobbies:	Classical music

*The author presented on this page has published more than **10 articles** in Angewandte Chemie in the last 10 years, most recently:* "Nanoindentation in Crystal Engineering: Quantifying Mechanical Properties of Molecular Crystals": S. Varughese, M. S. R. N. Kiran, U. Ramamurty, G. R. Desiraju, *Angew. Chem.* **2013**, *125*, 2765–2777; *Angew. Chem. Int. Ed.* **2013**, *52*, 2701–2712.

Chemistry is fun because … it is an assault on the senses!

My favorite quote is … "To strive, to seek, to find, and not to yield" from Tennyson's poem "Ulysses".

If I could be any age I would be … 60, which is my age at the time of writing.

My favorite time of day is … 9 a.m.

My favorite molecule is … benzene.

If I had one year of paid leave I would … resume learning Karnatic (South Indian classical) vocal music.

My favorite painter is … Diego Velasquez.

My favorite composer is … Muthuswami Dikshitar (1775–1835), one of the musical trinity of Karnatic music.

My favorite book is … Winston Churchill's "The Second World War, Volume 1: The Gathering Storm".

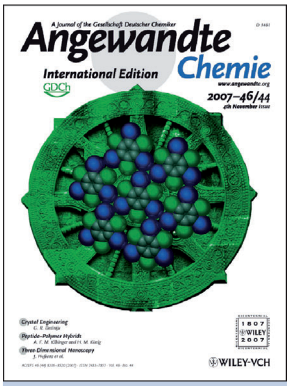
If I could be described as an animal it would be … a cat.

The biggest challenge facing scientists is … supplying clean drinking water for everybody.

The most significant historic event of the past 100 years was … the Second World War.

If I were a car I would be … a Premier Padmini (registration numbers TMR 9579 or AP9 796).

My first experiment was … actually successful.



The work of G. R. Desiraju has been featured on the cover of Angewandte Chemie: "Crystal Engineering: A Holistic View": G. R. Desiraju, *Angew. Chem.* **2007**, *119*, 8492–8508; *Angew. Chem. Int. Ed.* **2007**, *46*, 8342–8356.

How is chemistry research different now than at the beginning of your career?

Chemistry has not really changed, but the way we do research has changed. The most important difference is that getting money seems to have become a macho thing. The more money you get, the better assessed you are as a chemist. Students are also different. When I began my research in Illinois in 1972, there were 110 students in the first-year PhD class. They distributed themselves fairly evenly in the organic, inorganic, physical, and analytical sections of the department. Today, most students rush to certain subjects in the hope that their chances of getting a job will improve. Another big difference today is the role of the internet and other electronic media in obtaining information and reading the literature. When I was a student, I would read Chemical Abstracts (hard copy of course) regularly. Students remembered what they read, and covered many areas. Today, a student will download lots of papers, but only in a small specialized area that is important for his/her immediate project or manuscript.

What is the secret to publishing so many high-quality papers?

I don't really know. Quality is quality. You either have it or you don't. I do what I think is interesting and useful. I take up a certain line of research (for example my studies on the $C-H\cdots O$ hydrogen bond) when the literature appears to me to be totally confusing. I think if one identifies crucial gaps in an area, and starts filling them systematically and unemotionally, one could get a high-quality paper. Any area that resists easy classification is a fertile ground for research. When I began my independent research, both organic and physical chemists were clear that crystal engineering was not a part of their subject. Today, crystal engineering is a distinct subject and its practitioners are not concerned whether or not they are considered to be organic chemists or physical chemists by their departmental colleagues.

My 5 top papers:

1. "Supramolecular Synthons in Crystal Engineering—A New Organic Synthesis": G. R. Desiraju, *Angew. Chem.* **1995**, *107*, 2541–2558; *Angew. Chem. Int. Ed. Engl.* **1995**, *34*, 2311–2327.
   More than any other, it is this paper that characterizes my work, and by the time I finished writing it, I realized that the key to designing organic crystal structures lay in the retrosynthetic approach provided by organic chemistry, rather than the molecule→crystal approach through, say, atom potentials and computation that is derived from physical chemistry. I can safely say that my research career was never the same after I wrote this paper. Unlike many reviews that come after the event, this review was a blueprint for future work by me, and by so many others in the crystal engineering area.
2. "C–H···F Interactions in the Crystal Structures of Some Fluorobenzenes": V. R. Thalladi, H.-C. Weiss, D. Bläser, R. Boese, A. Nangia, G. R. Desiraju, *J. Am. Chem. Soc.* **1998**, *120*, 8702–8710.
   In this paper, we proposed that the weakest types of hydrogen bond, namely those formed by "organic" fluorine played a conclusive role in determining crystal structures. This paper was significant in that it provoked a long (and in hindsight largely unnecessary) debate with Jack Dunitz and Angelo Gavezzotti about the respective roles of chemical interactions and space-filling arguments in crystal packing, in other words about the significance of synthons themselves. I would say that this debate largely ended with our crystal-structure analysis of 1,2,3,5-tetrafluorobenzene (*CrystEngComm* **2010**, *12*, 2079–2085) and the paper by Dunitz and Gavezzotti (*Cryst. Growth Des.* **2012**, *12*, 5873–5877) in which they provided computational confirmation for the viability of almost all the supramolecular synthons supplied in my 1995 *Angewandte Chemie* paper. Our 1998 paper continues to be read and cited and scarcely a month passes before I see another paper on the C–H···F–C hydrogen bond.
3. "Distinction between the weak hydrogen bond and the van der Waals interaction": T. Steiner, G. R. Desiraju, *Chem. Commun.* **1998**, 891–892.
   This paper was written in unusual circumstances. A paper by Al Cotton and his associates (*Chem. Commun.* **1997**, 1673–1674) dismissed the idea of C–H···N hydrogen bonds in a derogatory manner and used outdated concepts of Pauling. Thomas Steiner and I decided that we would not respond in similar language but rather we provided evidence to show that the weakest kinds of C–H···O bonds formed by unactivated methyl groups still showed directionality that is absent in Me···Me close packing, in other words that they are hydrogen bonds. This paper silenced Cotton, and went on to become a rather highly cited contribution.
4. "Structural Studies of the System Na(saccharinate)·$n(H_2O)$: A Model for Crystallization": R. Banerjee, P. M. Bhatt, M. T. Kirchner, G. R. Desiraju, *Angew. Chem.* **2005**, *117*, 2571–2576; *Angew. Chem. Int. Ed.* **2005**, *44*, 2515–2520.
   This study was a remarkable experience. We obtained these hydrated crystals of a very common nutraceutical by accident. We found that the substance gains and loses water equally easily and quite rapidly depending on the ambient conditions. The crystal unit was large, messy, non-uniform, and highly solvated. We proposed that this structure is a good model for a crystal nucleus. The referees termed it a VIP paper. Roger Davey contests our interpretation in a recent Review in *Angewandte Chemie*, but it will still be a while, in my view, before anyone sees a crystal structure (which by definition corresponds to an energy minimum) that is this close to the energy maximum species that we call a crystal nucleus.
5. "Crystal Structures of Polynuclear Aromatic Hydrocarbons. Classification, Rationalisation and Prediction from Molecular Structure": G. R. Desiraju, A. Gavezzotti, *Acta Crystallogr. Sect. B: Struct. Sci.* **1989**, *45*, 473–482.
   How can I forget this paper? Angelo Gavezzotti and I had been working jointly, but each in our respective countries, with condensed aromatic hydrocarbons, for nearly four years, in the pre-e-mail era, and trying vainly to convince journal editors to publish this work that attempted to relate crystal structures with molecular structures. While many of the arguments used here will not work for more polar derivatives, and indeed this is what led me to thinking about synthons, I remember this paper because after it appeared, both the authors suddenly became well-known. Publication of a paper in a not-so-high-impact journal can certainly bring scientific recognition if the paper is good and timely. People read papers no matter where you publish them.

DOI: 10.1002/anie.201302516