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Fall Seminar Series

Why Are Crystals Straight?

Bart Kahr, PhD Professor **Department of Chemistry New York University** Wednesday, October 9, 2:00 p.m. **PISB 104**

In chemistry, we know the vast majority of what we know about molecular structure from the scattering of X-rays from crystals. Diffraction works so well because crystals have long range translational symmetry. In fact, crystals are straight, by definition. Their sharp edges and flat faces, so unlike most everything else in Nature, "flash forth their symmetry", according to Federov. Translational symmetry is first and foremost. However, we have shown in the past decade that a large fraction of simple molecular (organic) crystals can be made to grow with helicoidal morphologies, as structures with curvature that are decidedly not straight. This is an extraordinarily common fact about crystal form that is very easy to observe. We illustrate this with the four common over-the-counter pain medications: aspirin (Bayer), ibuprofen (Advil), acetaminophen (Tylenol), and naproxen (Aleve). It is incomprehensible that helicoidal crystals, as common as they are, remain unknown among the great majority of contemporary crystallographers. Nevertheless, the forces involved in twisting crystals have been difficult to identify. Studies of the mechanisms that give rise to these apparent distortions in crystals that twist as they grow has developed into a meditation and a program of computation aimed at understanding why and when crystals develop translational symmetry. We have come to see translational symmetry not as a requirement of crystallinity, but rather as an imperfect compromise between free energy and size.

Bart Kahr was born in New York City in 1961. He studied chemistry with I. D. Reingold at Middlebury College, with Kurt Mislow at Princeton University (Ph.D., 1988), and with J. M. McBride at Yale University. He was a faculty member at Purdue University from 1990 to 1996 and at the University of Washington, Seattle from 1997 to 2009. After which, he returned to his hometown where he is currently Professor of Chemistry in the Molecular Design Institute at New York University. Kahr's research group studies the growth, structure, and physical properties of complex organized media. Bart also practices the experimental history of chemistry and crystallography, that is those aspects of the development of science of can only be informed by contemporary laboratory experiments. In recent years, he has been advocating for the changes in the way that universities and government agencies manage scientific misconduct. Bart Kahr has published 245 papers and given as many invited lectures. In 2014, he was named NSF Distinguished Lecturer in the Mathematical and Physical Sciences.