



Ph.D. Course in Materials Science and Nanotechnology

University of Milano-Bicocca, Department of Materials Science, via Cozzi 55, 20125 Milano

October 18, 2019 – 2.30 p.m. Seminar room - Department of Materials Science U5

Bart Kahr

Department of Chemistry & Molecular Design Institute, New York University

Why Are Crystals Straight?

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.

PhD students and all interested in the seminar are kindly invited to participate.

The PhD Coordinator Prof. Marco Bernasconi