THE DEPARTMENT OF CHEMICAL ENGINEERING presents the

Distinguished Lecturer

Michael F. Doherty

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Tuesday, April 15, 2014

10:45-11:35AM in WEB L104

From Form to Function: Crystal Engineering for Organic & Drug Molecules

Abstract:

Crystalline organic solids are ubiquitous as either final products or as intermediates in the fine chemical, pharmaceutical, organic electronics, and home & personal care industries. In most cases the properties of the crystalline solid (e.g., structure, shape, size, etc.) have a major impact on the functionality of the product as well as the design and operation of the manufacturing process, and in most cases the two cannot considered separately. Gibbs was the first to recognize that crystals rarely achieved their equilibrium (surface energy minimizing) shape but it took almost 100 years to discover how to identify their real growth shapes. In this seminar I will describe a novel, (relatively) simple and accurate method for predicting the shape evolution and ultimate steady-state shape of 3-dimensional faceted crystals grown from solution. The model is initialized from an arbitrary initial seed shape and size, but known polymorph. The growth model for the crystal faces is based on the pioneering screw dislocation model of Burton, Cabrera and Frank in which surface integration kinetics is the rate determining step. The model has been successfully applied to a selection of complex molecular crystals of interest in pharmaceutical applications.

Short Biography:

Michael F. Doherty is Professor of Chemical Engineering and former Department Chair at the University of California Santa Barbara. He received his B.Sc. in Chemical Engineering from Imperial College, University of London in 1973, and his Ph.D. in Chemical Engineering from Trinity College, University of Cambridge in 1977. His research interests include process systems engineering with particular emphasis on crystal engineering, and separation with chemical reaction. He is the holder of four patents, has published over 200 technical papers and given over 250 invited lectures. He has received numerous honors and awards for his teaching and research, including the Alpha Chi Sigma Award for Chemical Engineering Research (2004) from the AIChE and the E. V. Murphree Award (2012) for Research in Industrial and Engineering Chemistry from the ACS. In 2008 he was named one of the "One Hundred Chemical Engineers of the Modern Era (post 1945) by the AIChE.

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