



## Mechanic Studies for Crystallizations with Polymers

### Vilmalí López-Mejías, PhD

Faculty of Natural Sciences, Dept. of Chemistry  
University of Puerto Rico, Río Piedras Campus

**Abstract:** The assembly of molecules into the solid state can be accomplished in a number of nearly isoenergetic ways, which differ mainly in the arrangement and/or conformation of the building units; a phenomenon termed crystal polymorphism. Polymorphism can influence numerous solid-state properties, such as color, stability, solubility, dissolution rate, vibrational and electronic transitions. The thermodynamically most stable form under ambient conditions is in many cases considered the most attractive crystalline form. This form has a lower tendency to transform during manufacturing and storage. A metastable phase is less likely to be commercially employed unless it offers a significant increase in product's performance. While defining the "desired" polymorph is a matter of perspective (and to some extent intellectual property rights), gaining access to different polymorphs and controlling their appearance requires an understanding of the fine interplay between thermodynamic and kinetic aspects driving the crystallization. This talk focuses how our research is helping the scientific community gain fundamental understanding for the different scenarios in which pharmaceutical crystals form. Particularly, we will discuss how heterogeneous nucleation processes and phase transitions enable the control over polymorphism in polymer-based drug formulations. Mechanistic studies for three different crystallization processes (solution, sublimation, and melt) will be discussed in model pharmaceutical compounds (flufenamic acid, tolfenamic acid, and acetaminophen) in the presence of various polymers. The implications of this research transcend beyond pharmaceutical compounds and can be applied across a wide range of materials with commercial interest such as electronics, energetics, and agrochemicals.

**Biography:** Dr. López-Mejías' research is focused on the crystallization of pharmaceutically active compounds with emphasis on the design of novel crystalline forms (i.e. polymorphs, cocrystals, salts) and polymer-based formulation strategies that enable an improved pharmaceutical performance. Her specific areas of expertise include: (1) solid form discovery and control through directed molecular interactions at tailored polymer-solute interfaces, (2) development of tailored polymeric (nano)formulations for insoluble compounds, and (3) mechanistic understanding of the molecular level interactions leading to polymorph formation in polymer-based formulations. The goal of her research activities is to provide a comprehensive scientific basis for the successful application of alternative polymer-based solid dosage formulations (i.e. hot-melt extrusion, additive manufacturing). The implications of this research interests transcends beyond pharmaceutical compounds and can be applied across a wide range of materials with commercial interest (electronics, energetics, agrochemicals, etc.).

In the short span of her academic career Dr. López-Mejías' has authored 12 publications, 2 book contributions, and is an inventor on 2 patents. She is a reviewer for the American Chemical Society Journals, *Crystal Growth & Design*, *Analytical Chemistry*, and *Journal of Chemical & Engineering Data* and Royal Society of Chemistry Journal, *Crystal Engineering Communications*. She is an invited member of the *Engineering Research Center for Structured Organic Particulate Systems (C-SOPS)*, and *Institute of Functional Nanomaterials (IFN)*. She forms part of several NSF funded centers; Center for the Advancement of Wearable Technologies (CAWT), Center for interfacial electrochemistry of energy materials (PREM-CiE<sup>2</sup>M), and the Wisconsin - Puerto Rico Partnership for Research and Education in Materials [Wi(PR)<sup>2</sup>EM].

Materials  
Engineering  
MSE 690  
Fall 2019  
Seminar Series

Friday, Oct. 4th  
Snacks 3:30 pm  
Presentation 3:45 pm

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