# BI-CO MATHEMATICS COLLOQUIUM


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## "Modeling the 'Cambrian explosion' of Topological Polymers"

**Monday, October 1, 2018**
Talk at 4:00 – Park 338
Tea at 3:30 – Park 361, Math Lounge


**Abstract:**
Polymers-- macromolecules composed of long chains of similar elements-- are a fundamental component of our world. They make up our clothing*, our housing**, our food***, and even ourselves****! Classical synthetic polymers are ``linear polymers" with two free ends. Ring polymers, where the two ends of the polymer are bonded together to make a loop, represent a 21st century advance in synthetic chemistry, with a variety of appealing (and really different) physical and chemical properties.

Very recently, new advances in synthetic chemistry have enabled the synthesis of polymers with more graph types-- polymers with the structure of a tetrahedron, for instance, or a theta-curve, or a complete bipartite graph. So many new polymer topologies are being synthesized at such a rapid rate over the past few years (2016-2018) that chemists describe it as a "Cambrian explosion" of topological polymers. The new polymers seem to have fascinating and previously unseen properties, which hold out promise in technology, energy, and medicine.

In this talk, we present a model for these topological polymers as Gaussian random walks whose overall topology is constrained by any (arbitrary) graph G. It turns out to be the case that understanding the constraints comes down to a mixture of topology and linear algebra, and that the model ties into some rich mathematics connecting graph theory and chemistry from the 1990's. We'll present an algorithm for sampling configurations of these polymers, as well as some theoretical results. In particular, we'll give a nice formula for the expected radius of gyration of a topological polymer in terms of the eigenvalues of the graph Laplacian of the underlying graph G.



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* nylon, Kevlar
** polystyrene, polypropylene, teflon
*** jello, gluten, glycogen, cellulose, starch
**** DNA, RNA, proteins

**BRYN MAWR COLLEGE**