



Paulo Henrique Santos received both his BS in Food Engineering and MS in Chemical Engineering from University of Campinas (UNICAMP), Sao Paulo, Brazil. In 2008 he joined Dr. Campanella's group as a Ph.D. student to work on a multidisciplinary project on hypergolic gels funded by the U.S. Army Research Office under the Multi-University Research (MURI). His research at Purdue combines both experimental (rheology) and theoretical work (focusing on molecular dynamics simulations).



Dissertation Defense

Speaker: Paulo H. Santos

Title: Mechanical Characterization and Computational Modeling of Gels

Major Professor(s): Osvaldo H. Campanella

Date: Monday, November 21, 2011

Time: 10am

Location: NLSN 2187

Abstract:

Gels are of great importance in many different areas such as chemical, cosmetics, pharmaceutical and food. Even though gels are present in our daily basis, the gel state is easier to be recognized than to be defined. It is still a challenge to link macroscopic properties of materials with their microstructural properties and conformation. In practice, macroscopic properties of gels provide important and useful inputs to the design of new materials. From the experimental point of view, the objective of my research is to use appropriate constitutive equations that describe the rheological behavior of complex systems, taking into account the combined effects that may describe different types of gels produced by different processes. However, given the large number of variables it is very difficult to only experimentally establish the relation between the individual components of the system, the resulting microscopic structure and the final macroscopic properties. Computer simulations offer the opportunity to bridge this gap, and allow the exploration of new applications for polymeric and particulate systems. Molecular dynamics and Brownian dynamics can be used to simulate the gelation process and to calculate the mechanical properties of the resulting systems.

Application:

Suitable predictive molecular models provide guidelines for the design of new materials tailoring specific applications.