## **Physics Department Colloquium**

## Dr. Joseph L. Baker

## **Department of Chemistry, TCNJ**

Title: Biomolecules in Motion: Molecular Modeling and Simulation of Biomolecular Systems

Abstract: Molecular dynamics simulation allows for the study of the motion of bio-molecular systems at a level of detail that is unachievable using experimental methods. At its core, the method propagates the motion of atoms through time by invoking Newton's Second Law to calculate the forces between a large number of atoms, and then leveraging high performance computing resources to iterate these calculations many millions of times. Therefore, simulated models can be used to directly probe the underlying chemistry and physics of bio-molecular systems at an atomistic level of resolution, providing novel insights into bio-molecular dynamics and function. In this talk, I will introduce the molecular dynamics method, and will discuss the applications of modeling and simulation to several systems of current interest in the Baker lab, including bacterial filaments and motors, ionic liquids and lipid membranes.

Date: Friday, November 20, 2015

Time: 12:30 PM

Where: Science Complex, P-317