

Department of Physics

McMicken College of Arts and Sciences

**SUMMER RESEARCH OPPORTUNITIES  
FOR UNDERGRADUATE WOMEN**

**APPLICATION DEADLINE: March 1, 2007**

*The Department of Physics is pleased to offer the following research project for the summer of 2007. Interested students are urged to contact the faculty member(s) directing the project that most interests them. By contacting the faculty member, you can discover more about the project, learn what your responsibilities will be and if possible, develop a timetable for the twelve-week research period.*

**COMPUTATIONAL INVESTIGATIONS OF TRANSITION STATES IN  
CHEMICAL REACTIONS**

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**Project Description**

The goal of this research is to develop a computational tool that can uncover the pathway and the transition states that exist when a molecule changes conformation or when it chemically changes. In such circumstances, a process must overcome an energy barrier before proceeding to completion. If the size of the barrier is large compared to the available thermal energy, a process must rely on the occurrence of one or more rare events. For such circumstances, one would like to understand the reaction pathways so as to improve yields, or as in the case of protein folding, to understand the intermediate steps. Many simple processes have been explored using theoretical tools such as molecular dynamics, where the movements of individual atoms are calculated. However, when the barrier is large, crossing the relevant barrier is indeed a very rare event. Although computer speeds have been doubling every 18 months (Moore's law), the exponentially long waiting times necessary for barrier hopping pushes the required computational effort out of the feasibility range for all but the simplest models. To explore these barrier-limited processes, a novel computational technique called Transition-Path sampling, has been developed. The summer student will learn some of the (mathematical) background of this technique, will help further develop the implementation of this technique, will apply this method to some simple systems, and will assist in analyzing results.