499Enrollment Form

Check all that apply: _____ 499 A ___X___ 499 B ___X___ 499C

Please type your responses using an electronic copy of this form. Contact Joy Drinnon for a copy or visit the Office of Undergraduate website.

Enrollment Term and Year: Summer 1969

Student Name(s) and Contact Info: Iva G. Reatmind

Faculty Mentor(s): Dr. U. Doolittle

Student Major and Expected Graduation Date: Chemistry, Mathematics; May 1971

Desired prefix for this 499 (e.g., BIBL, HUMN, PSYC): PHYS

Relevant Prerequisite Courses/Experience: CHEM 170, 171, 301, 302; MATH 211, 212, 303; PHYS 203, 204; CIS 211, 297

Anticipated Expenses or Special Equipment Needs: Research workstation (potentially); see proposal

Planned research activities (499A): *Please attach a list of research activities you and your mentor plan to do this semester.*

Research Proposal (499 B)**:** *Please attach a typed research proposal which follows the attached guidelines.*

Conference Plans (499C only): *Please attach a description of any conferences or journals where you hope to share you research. Please attach a copy of an abstract and bibliography of your research thus far. (Note: The committee may request additional information if this is a new project and you do not already have a 499B proposal on file with the Office of Undergraduate Research.)*

Student's Signature:_____

Mentor's Signature:_____

Area Chair's Signature:_____

Director of UR Signature:_____

499B Proposal

Partially Ordered Phases of Mixed Alkanes

Section 1: INTRODUCTION AND PURPOSE OF THE STUDY

Rotator phases of *n*-alkanes provide an interesting example of a partially ordered solid phase, with molecules in organized positions like in a crystal but free to rotate in place. Overall properties of alkane rotator phases have been studied extensively in experiments on many lengths of alkane [1]. The behavior of individual molecules in a rotator phase has been studied through computer simulations. [2] Some theories suggest that rotator phases are involved in the formation of polymer crystals, which makes the understanding rotator phases potentially valuable to industrial polymer science and technology. [3] The purpose of our research is to examine through computer simulation the effects of bidispersity of alkanes on the crystal and rotator phase properties, which has not been studied extensively before.

Section 2: STATEMENT OF THE PROBLEM

Experiments have indicated that rotator phases behave differently in mixtures than when all alkanes have the same length. Specifically, the rotator phase is found over a larger temperature range for a binary mixture than for a pure sample [2,4]. Previous simulations tested only one binary mixture and found an expanded temperature range. [2] We will examine the overall phase behavior of several binary mixtures, to compare to experiments. We will also examine the behavior of individual molecules to determine a cause for the changes in behavior of the material.

Section 3: APPROACHING THE PROBLEM

We plan to perform our molecular dynamics simulations using the GRAOMCS molecular simulation package. We will also need to program our data analysis tools (using C++, Python, etc.) to analyze the simulation output.

Current computational resources for students to use for data analysis are limited, so we may need to obtain a desktop workstation for student use in one of our labs. The estimated cost is $2500.

This project is part of an ongoing research program and is not expected to be publishable by itself. However, the results may be suitable for a poster presentation at a regional or national meeting on physics or polymer science.

Section 4: PRELIMINARY REVIEW OF THE LITERATURE

[1] Sirota, E. B., et al, *J. Che.m Phys*. **98**:5809 (1993)
[2] Wentzel, N. and Milner, S. T., J. Chem. Phys. **134**:224504 (2011)
[3] Milner, S. T., *Soft Matter* **7**:2909 (2011)
[4] Herhold, A. B., et al, *J. Chem. Phys.* **116:**9036 (2002)

499C SAMPLE ABSTRACT

Abstract:

Urate Oxidase from \textit{Asperigillus flavus} has been shown to be a model protein in terms of understanding the effects of PEG on the crystallization of large proteins. Extensive experimental studies based on SAXS (Vivares et al, J. Phys. Chem. B 108, 6498 (2004)) have determined the effects of salt, pH, temperature, and most importantly polyethylene glycol (PEG), on the crystallization of this protein. Recently, some aspects of the phase diagram have also been determined. In this paper we use Monte Carlo techniques to predict phase diagrams for urate oxidase in solution with PEG. The model used includes an electrostatic interaction, van der Waals attraction, and a polymer-induced depletion interaction (Vivares et al, Eur. Phys. J. E 9, 15 (2002)). Results of the simulation are compared with experimental results.

Bibliography

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Y. Choi, T. Ree, and F. H. Ree, J. Chem. Phys. 95, 7548 (1991).
A. M. Ferrenberg and D. P. Landau, Phys. Rev. B 43, 5081 (1991).

SAMPLE 499C

Conference Plans and Anticipated Expenses

We hope to present our results as a poster at the American Physical Society March Meeting in Baltimore, MD, held from March 13 to March 17. Registration costs are $360 for Dr. Doolittle and free for Iva. Anticipated hotel expenses in the Baltimore area are $260 per night for our group (one professor, two students; we would need two rooms for Dr. Doolittle and Iva), and we expect to stay three nights, March 12, 13, and 14. Air travel plus local transportation from TRI to BWI or DCA is a prohibitively expensive at $500 per person for Iva and Dr. Doolittle, so we plan to drive. The round trip from Milligan to the conference is 904 miles, which at the current GSA rate of $0.565 per mile is $510.76 round trip. Meals are not covered in the conference fee; expected meals and incidentals per diem is $40 per person for Iva and Dr. Doolittle (lower than the GSA rate but realistic based on Dr. Doolittle's experience). Total cost for the trip is estimated at about $1730. Prepayment would be required only for Dr. Doolittle's conference registration, if actual receipts are desired.