James T. Kindt
Assistant Professor, Department of Chemistry
Emory University, Atlanta, Georgia 30322
tel: (404) 712-1817 e-mail: jkindt@emory.edu

December 7, 2004

James Musser, Chair
Department of Physics
Indiana University
727 E. Third St
Bloomington, IN 47405-7105

Dear Professor Musser and members of the search committee:

I am pleased to offer my enthusiastic recommendation for Dr. Jason de Joannis for a faculty position at Indiana University. Jason was the first postdoctoral fellow to join my group; I arrived at Emory in the Fall of 2001, and he arrived in July of 2002. I was familiar with his work in Mainz on electrostatics calculation methods, having heard it praised by a colleague who is an expert in that area, so I was surprised and delighted when he expressed interest in joining my fledgling group. Jason had family reasons for wishing to be in Atlanta at the time, and desired to gain exposure to biomolecular simulation methods.

Jason's main project has been development and implementation of new methods for modeling mixed-lipid bilayers using configuration bias Monte Carlo. The project goal is to address a longstanding biophysical problem and a major challenge in molecular simulation of lipid bilayer membranes: determination of the equilibrium lateral distribution of different kinds of lipids in a mixed-lipid membrane. The lateral diffusion of lipids is too slow to observe equilibrium mixing during a feasible molecular dynamics simulation run of 10's of nanoseconds. Jason has developed "alchemical" biased chain re-growth moves to change lipid type; implemented with the proper acceptance probabilities, these moves can be used to simulate equilibrium mixing of different components of the membrane much more efficiently than by following realistic dynamics.

Jason quickly picked up the ins and outs of the molecular force-field our group was using, wrote the computer code that generates the moves and determines the acceptance probabilities, and completed a series of proof-of-principle calculations to show that the method should work efficiently. He has nearly completed the implementation of this method within the Gromacs molecular dynamics simulation package, an accomplishment that required a deep level of understanding of very complex software and creativity in engineering an interface to his own code. I consider it a strategic management failure on my part, and not any reflection on Jason's skill and hard work, that this project has yielded few publishable results. I regret not initially encouraging him to pursue smaller side projects with a shorter horizon.

Beginning in the Spring of 2004, Jason has taken on three such projects. He is working with a graduate student in my group on simulations of lipid and surfactant mixtures using less detailed molecular models; he oversaw the work of a visiting graduate student from Brasenose College, Oxford investigating the mechanical rigidity of lipid bilayers, and is also guiding an organic chemistry student with her first computer simulations of a class of amphiphilic molecules that she has synthesized. His input has been key in all of these cases, and I expect at least three solid papers to come out of these efforts.

While working on these projects, Jason has gained a good deal of experience in biomolecular simulation methods, while demonstrating sound expertise in physical theory and mathematics, and excellent skills in general problem-solving. He has consistently shown interest in expanding his understanding of areas, like cell biology and quantum chemistry, that were not emphasized in his previous education. I should add that although I provided the initial ideas and have offered general guidance in his work, he has been completely independent in the execution (as well as in the development of the research proposal he submitted for job applications). He has been an asset to my research group in many ways going beyond his own project, particularly in giving advice to graduate students and in contributing to the management of our computer systems, where I often rely on his judgment. Jason is fully prepared to lead a research group himself. He is polite but not timid, and I think he would be an able leader within his group and a responsible and valuable colleague within the department.

Jason is a natural and enthusiastic teacher, both formally and informally, and I have been very pleased with the reports I've had from my classes when I have asked him on two occasions to substitute for me in courses on thermodynamics (undergraduate physical chemistry) and statistical mechanics (first-year graduate physical chemistry). My sense is that he truly enjoys teaching. Jason frequently asks good questions in departmental seminars, and serves as a personable host for visiting speakers, who in our department are traditionally taken to lunch by graduate students and postdocs. Furthermore, the synthetic organic chemistry student he has been helping has spoken of his mentorship abilities in the most positive possible terms.

Based on his intellect, skills and experience, I believe that Jason has excellent potential to develop an internationally known, well-funded basic research program in theory and simulation of biopolymers, lipids, and other systems of biophysical importance. If I can be of further assistance to the committee, please do not hesitate to contact me.

Sincerely yours,

James Kindt