Dear Dr. Musser,

It is a pleasure for me to write a letter of recommendation for Dr. Jason L. de Joannis for his application for a faculty position in the Department of Physics at Indiana University.

Dr. Jason de Joannis was part of my group from November 1, 2000 - May 2002. My subgroup, see i.e. http://www.mpip-mainz.mpg.de/~pep, is one of eight in the theory group which are all headed by a group leader like myself, and perform independent research on all theoretical aspects of polymers. The whole theory group is directed by Prof K. Kremer.

Dr. de Joannis' overall project was concerned with simulations on free standing polyelectrolyte films, where experiments observed unusual film thickness jumps in the thin films on varying the external pressure. These are theoretically not understood. One conjectures that the thickness jumps are of the order of the correlation length (mesh size) in the semi-dilute polyelectrolyte solution, however there is no microstructural understanding of this behavior.

We were trying to model the polyelectrolyte solution in a thin film on the basis of charged bead-spring model where we explicitely take the counterions into account. In this case the periodic boundary conditions apply only to 2 dimensions, and the third one is finite. This poses extra difficulty on the proper treatment of the long range interactions when the Ewald sum is performed. For this purpose he and A. Arnold (a ph.D student of mine) have recently developed a simple method (ELC) by which one uses the 3D Ewald sum plus a layer correction term, which eliminates the influence of the unwanted replicas. By this simple trick, one can still use advanced 3D algorithms like the particle mesh Ewald methods (P3M) which have a favorable scaling for N charges (N log N) compared to ``classical'' 2D methods which go typically like $N2$. This algorithm has been described in two papers in J. Chem. Phys., and Dr. de Joannis is the first author of the second one, describing its practical applications.

Dr. de Joannis has developed the full details of how to compute the thermodynamic pressure tensor, which also is very non-trivial due to the complicated mathematical form of the correction term in the ELC method. We have already seen some unusual behavior, but needed more simulational data to interprete our preliminary results. Unfortunately Dr. de Joannis left before we could finish that part, but we are still collaborating on that subject. In fact he just visited us this summer, and we are just about to finish our paper with very nice results.

Dr. de Joannis is definitely a very dedicated scientist who has the ability to learn new techniques and apply them to various problems. Although he had never worked on MD simulations before, and had also no particularly knowledge about the intricacies of long range interactions, he learnt very fast the essential concepts. He is very independent and comes up with suggestions on his own on how to attack the problem. He is very thorough in his investigations, and definitely wants to understand the basic facts of the problem he is working on. He has excellent numerical and computational skills and can convert the scientific demands into executable programs. He also independently handles the reading the relevant background literature in theory and experiments. In

fact, I was quite surprised about his intellectual breadth, which changed my attitude towards chemical engineers. He had very good communicative skills and interacted freely and independently with the other scientists here in my group, but also outside of it.
Since the problems he has and is working on are ones of very basic interest, I do not expect that he will have great difficulties in attracting sufficient funding for his research, either at NSF, NIH, DOE, or similar institutions.

I do not hesitate to recommend him strongly for the faculty position, and I am sure he will significantly strengthen the Department of Physics at Indiana University.

With best regards

Dr. Christian Holm

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