FOUNDATION FOR RESEARCH AND TECHNOLOGY - HELLAS (FO.R.T.H.)

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Dr. Jason de Joannis was the last of my doctoral students in the Dept. of Chemical Eng. at the University of Florida. His Ph.D. research was conducted during the period of my transition from the University of Florida to the Foundation for Research and Technology, Hellas (FO.R.T.H. in Heraklion, Crete, Greece). As a result of these special circumstances, Jason received the least direct guidance by me and assumed the most responsibility for a successful completion of his dissertation among any of my past students.

Jason's dissertation constituted a systematic test of existing theories on the conformations (statistical thermodynamics) of polymeric molecules physically adsorbed on solid substrates. Furthermore, his dissertation explored the related consequences on the distance dependence of *steric forces between solid substrates coated by physisorbed polymers*. To this end, it quantified the effect of relevant material properties (physical chemistry of polymer, solvent and substrate, as well as molecular weight of adsorbed chains). These issues are central to the stabilization of colloidal dispersions and material property control of various polymeric coatings (with applications in microelectronics and nanotechnology).

Jason employed and developed advanced molecular simulation techniques (initiated by D. Frenkel & coworkers, FOM, The Netherlands), in order to test *quantitatively* existing theories on physisorbed polymers proposed in the late 70's and early 80's (Scheutjens and Fleer, de Gennes) and extended in the mid 90's (Semenov, Joahny). Experimental tests, employing neutron reflectivity and SANS did not and, even today, *do not* have the sensitivity

to distinguish between competing (and often conflicting) theoretical predictions. Therefore, 'computer experiments' were the only tool that allowed *direct and quantitative* testing of the above theories. Although competing theoretical predictions existed since the early 80's and the experimental (ambiguous) tests appeared in the late 80's and early 90's, no simulation effort had addressed satisfactorily these issues. This state of affairs underscores the difficulty of the whole endeavor.

During the last two years of his Ph.D. research Jason expanded, *on his own initiative,* the scope of his research. He developed a close collaboration with Dr. J. Jimenez (then a Ph.D. student of Raj Rajagopalan). Jason and Jorge combined the simulation methodologies they had developed (Contact Distribution Method and Random-End-Switching Configurational Bias Monte Carlo). They, for the first time, calculated the forces between solid surfaces confining nanoscopically thin films of polymer solutions. This effort allowed a direct comparison with relevant AFM and SFA (surface force apparatus) experiments. Furthermore, these simulation studies demonstrated the severe quantitative limitations of mean-field approaches and offered insights on the range of validity of scaling approaches. It seems that when Jason was exposed to laboratory experiments (AFM) and *actually did some,* he came out with fresh ideas and initiatives on how to pursue the problem on the computational front.

In the final months of his Ph.D., while supervising an undergraduate student, Jason offered substantial help in the development of a hard-sphere Monte Carlo code that can handle about 30,000 particles on a desktop PC. His contribution boosted the project of my first Ph.D. student at FORTH-IESL.

After the completion of his Ph.D. work, Jason, on my advice, sought a post-doctoral appointment at the Max-Planck Institute for Polymer Research (Mainz, Germany). He worked on state-of–the-art methodologies for the simulation of polyelectrelolytes and optimal algorithms for Ewald summations of charges in thin films. Polyelectrolyte adsorption is more complicated than that of uncharged polymers. The thin-film Ewald summation (now published) represents a novel mathematical result and leads to the fastest available method O(NlogN). It should be the method of choice for many-particle simulation of charged layers. The above methodology was applied to soap films containing polyelectrolyte molecules. Jason's work demonstrated, for the first time, the presence of structural oscillations commensurate with film thickness and consistent with the scaling concepts of polyelectrolyte solutions. His simulation work pushed the frontier and expanded the horizon of our understanding in a problem whose physics is still incompletely understood and controversial. Jason pursued once more a rather 'hairy' problem, of the uttermost practical importance.

Jason is now extending his abilities in the biological front. In this effort he has employed an advanced MCMD (mixed Molecular Dynamics Monte Carlo) methodology in the 'semi-grand ensemble' context that allows for 'mutation moves' (i.e., Monte Carlo actions that alter the identity of atoms). This work gives insight into microscopic domain formation and elucidates the role of lipid distribution/membrane composition in major biological functions such as recognition, selective transport and cell fusion. In this problem subtle differences in molecular structure can have significant consequences on miscibility. Therefore it should be addressed, and is by Jason, at an *atomistic* level. To my knowledge, no atomistic simulation has succeeded in overcoming the bottlenecks in 'surface' diffusion. Jason's effort is very promising in this regard.

Jason served as a regular Instructor in one of the ChE department's entering courses (Summer 1999, the first course on Thermodynamics with an attendance of more than 50 students). He had already undertaken a substantial portion of substitute teaching for Thermodynamics II (Phase and Chemical Reaction Equilibria; Spring 1999). Student evaluations, in both cases, were enthusiastic. I am aware that he has lectured extensively both

in undergraduate Physical Chemistry courses and graduate Statistical Thermodynamics courses (focusing on advanced and rather delicate topics), while at Emory University. Jason's communication skills are excellent. He has presented several papers in major conferences (AIChE, ACS, APS) and has given many seminars in Academia and research labs. All were professionally prepared and delivered in the typical calm, secure and organized manner that characterizes his work in general.

Jason worked on a very demanding, and literally difficult, Ph.D. project under harsh circumstances. Not only did he meet the original goals, but he expanded the scope of the project and accomplished more. Jason always adopted a positive viewpoint. I am impressed by his capacity to overcome difficulties and *his ability to generate opportunities*. Jason has a remarkable depth and breadth of knowledge: Polymer Physics, Statistical Mechanics, and Molecular Simulations of a wide variety, a firm Chemical Engineering background and a substantial exposure to Materials Science and Bio-Science.

Jason de Joannis has been the best among my graduate students. Ranked on a scale broader than that of the University of Florida and including my 'alma mater' (University of Minnesota) he ranks comfortably among the top 5% of graduate students. He is a very intelligent, hard-working, ambitious, mature and collegial young scientist. All these qualities, along with his calm perseverance and intellectual breadth, will allow him to become a leader in his research field, someone who will open new avenues and expand horizons. Dr. Jason de Joannis has my strongest recommendation for an Assistant Professor position in your Department.

Sincerely,

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Principal Researcher
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