University of Illinois
at Urbana-Champaign

Beckman Institute
405 N. Mathews
Urbana, IL 61801

Klaus Schulten, PhD
Tel: (217)244-1604
Fax: (217)244-6078
Email: kschulte@ks.uiuc.edu
WWW:http://www.ks.uiuc.edu/

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Bio-complexity Faculty Search Committee
c/o Prof. Rob de Ruyter van Steveninck
Department of Physics
Indiana University
Swain Hall West 117
Bloomington IN, 47405-7105

Dear Professor de Ruyter van "Steveninck:

Dr. Aleksei Aksimentiev is an extraordinary young researcher who comes along only every decade. I can recommend him to your department with greatest enthusiasm and without hesitation.

Dr. Aksimentiev joined my laboratory as a postdoc after already impressive achievements from his thesis research and from previous postdoctoral work. Dr. Aksimentiev received his Ph.D. in chemistry, applying methods of field theory to characterize conformations of single macromolecules in dense polymer mixtures near a phase transition. He investigated self-assembly of gradient copolymer melts, computing, for the first time, the phase diagrams of these novel materials. He also developed an efficient method for simulating diffusion of surfactants on curved periodic surfaces. The impressive results for a single thesis are all characterized by a very high standard in theory.

During his postdoctoral work at Mitsui Chemicals Dr. Aksimentiev continued to study blends of polymers, focusing on the dynamics of phase transitions. Using conceptually demanding tools of computational geometry he analyzed properties of the patterns emerging from the phase transitions and discovered a scaling law for the connectivity of such patterns. He determined the threshold composition for a binary liquid mixture, which ensures a bi-continuous morphology of the phases resulting from the phase transition. Again he employed conceptually advanced mathematical methodologies that are perfectly suited for the problem investigated, but are rarely used by other physical science researchers.

When Dr. Aksimentiev carried out his work in my laboratory he excelled again in a novel approach applied to a very demanding research problem, the mechanism of torque generation in F0 ATPase. My group's molecular dynamics methods are limited to nanosecond time scales that are too short for the overall functioning of the F0 motor driven by a proton current. Dr. Aksimentiev opted to do both a molecular dynamics simulation and mathematical modeling, the former providing information on the elementary steps for the latter, the latter covering the entire time domain of Fo function. The research, that will appear in print in Biophysics Journal along with a briefer treatment in Adv. in Protein Chemistry, encompassed the most demanding molecular modeling study accomplished so far in my group. It involved first the building of the entire Fo ATPase structure from structural components, work of nearly two years. It involved then the mechanical testing of the hypothesized elementary steps of the motor. It also involved characterizing the microscopic properties of the steps deemed right and essential, e.g., through computationally determined friction constants. Finally, it involved the formulation of astochastic

model, its solution, and verification. We opted to publish this monumental work in Biophysics Journal since we did not find a good fit in other journals due to size limitations. Dr. Aksimentiev has repeatedly been invited to speak on the work already and was met with great enthusiam by the cognoscenti. I expect will lead to two further publications shortly. I add that the work was carried out in close collaboration with Professor Fillingame of the University of Wisconsin, a world leader in the Fo ATPase field.

Most recently, Dr. Aksimentiev engaged into a fascinating new experimental-computational collaboration, the development of nanopores for single molecule electronic measurements. The work is still in its infancy, but one can state that it has a huge potential. The development is based on silicon nanotechnology applied by a leader in the field, Greg Timp, Professor of Electrical and Computer Engineering at our university. The Engineers have produced, using highly focused electron beams as they arise in electron microscopy, pores that are as small as a nanometer in diameter and imaged their profile. They have then measured single molecule conduction events of single and double stranded DNA of various lengths and base pair composition. The events are characterized by reduction of ion currents during the occlusion of pore by the various DNA strands together with the conduction of the strands themselves, the latter driven as the ionic current by an applied voltage and the inherent negative charge of the strands. Dr. Aksimentiev has accompanied the development of the pores and, in particular, the interpretation of the current traces observed through simulations of the silicon pores in an ion bath with single DNS strands. The simulations clearly show the details of pore occlusion, ion conduction, and final strand conduction that already corresponds well to the observations, the time resolution is being pushed down to the near nanosecond limit of the simulations. The calculations of Dr. Aksimentiev require him to represent various silicon materials, e.g., silicon nitrate, along with the pore as well as a proper surface representation of the material in the pore lining, the ion bath, and the DNA strands. Simulations need to cover many nanoseconds and required a dedicated section of 256 processors for several months on the fastest machine of the US NSF centers. Such extraordinary calculations can be handled reliably only by outstanding experts in computational science like Dr. Aksimentiev. The results promise to revolutionize modern biotechnology through the use of man-made pores that are much more robust and adjustable than the biological pores used presently in another technological approach to single molecule electric recordings.

Dr. Aksimentiev is a first rate lecturer and a great group member. He can express himself extremely well in lectures as he proved numerous times in seminars and conferences. He collaborates well with others in the academic community as he proved in two large collaborative projects, one on F0-ATPase and one on nanopore single molecule recording. He has the great strength of combining a strong conceptual foundation in chemical physics and a rare expertise in computational science with a strong interest to collaborate on real systems with leading experimentalists.

In summary, Dr. Aksimentiev is a rare candidate that you will not often find in a whole decade worldwide.

I would be most happy to assist you with further information on Dr. Aksimentiev.

With best regards,

Klaus Schulten
Swanlund Professor of Physics