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Dear Members of the Search Committee,

It gives me great pleasure to recommend **Dr. Andriy Baumketner** for a faculty position in your department.

Andriy has a rich and diverse background in theoretical and computational physics. He received a formal training in condensed matter physics during his doctoral studies at the National Academy of Sciences of Ukraine (ICMP), where his research focused on a theoretical study of the dynamical properties of complex liquids. His first post-doctoral position was under Prof. Hiwatari in the Department of Computational Sciences at Kanawaza University. There, his research shifted to the computational study of biomolecules, with an emphasis on molecular dynamics simulations of protein folding. Andriy joined my group at UCSB in August 2002, where he has continued his research in the field of biophysics. Andriy is a prolific and independent researcher, who has taken a leadership role in my group, serving as a mentor to two graduate students. Andriy has superb analytical and computational skills and has made a number of important research contributions during his post-doctoral stay in my group. He has co-authored nine publications in the last two years, with several more in preparation. Andriy has worked on a number of problems in my group, including the nature of the glass transition in protein folding, the identification of improved reaction coordinates for folding and the helix to coil transition using different solvent models. I will focus here on his contributions in two areas, chaperonin-mediated protein folding and peptide aggregation.

Chaperonins are large biomolecules that assist the folding of proteins that are unable to fold on their own. The mechanism by which chaperonins increase folding rates and yields remains an important and unanswered question. Andriy developed a new computational model to describe the folding of a protein in the presence of a chaperonin and his simulations have suggested a novel mechanism to explain recent experimental results. He showed that folding rate enhancements are the result of the formation of a new

intermediate state in which the protein is bound to the chaperonin wall. This state offers an alternate, energetically more favorable, pathway to the folded state. This work was published in two leading journals, the Journal of Molecular Biology and the Proceedings of the National Academy of Sciences.

His second main area of research is in the development of computational models to understand the kinetics and thermodynamics of peptide aggregation, with an emphasis on the aggregation process involved in Alzheimer's disease. A hallmark of this disease is the presence of insoluble fibrils in neurons, resulting from the aberrant aggregation of Amyloid beta (Aβ) peptides. These large insoluble fibrils, as well as smaller soluble aggregates of (Aβ) peptides, appear to be toxic to cells and responsible for the neuronal degeneration observed in Alzheimer patients. Using a replica exchange molecular dynamics sampling protocol, Andriy has been able to characterize at a microscopic level the conformations adopted by (Aβ) peptides in solution. This is a major breakthrough as his simulations have provided the first atomistic description of theses peptides (JACS, in press; Biophys. J., submitted). Andriy has also investigated the aggregation of fragments of the (Aβ) peptides (Biophys. J., submitted) and his studies have provided new insight into the nature of the free energy landscape for aggregation.

I am confident that Andrij will be very successful in leading an active research group at the forefront of biophysical research in protein folding. In addition, he is a clear and enthusiastic lecturer and will make a first-rate teacher in the classroom.

Please do not hesitate to contact me if you have any questions.

Sincerely,

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