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Letter of Recommendation for Dr. Mohammed Reza Ejtehadi applying for Faculty Staff Position

Dear Prof. van Steveninck:

Dr. Ejtehadi was working in the Theory Department of Max Planck Institute for Polymer Research from November 1999 through September 2002. The Theory Group is imbedded in major activities on synthetic and biological macromolecules ranging from synthetic chemistry all the way to theoretical physics of such systems. Similarly the activities of the Theory Group itself range from theoretical chemistry like calculations (quantum chemistry, force-field calculations) all the way to macroscopic description of materials employing hydrodynamic theories. Within these activities a major effort is related to multiscale modeling of macromolecular materials. Although we so far, mostly devoted our effort to synthetic "soft matter", meanwhile such methods have also been applied to biopolymers, most notably DNA. This activity within our group was headed by Dr. Ralf Everaers who has a long standing experience in computer modeling of polymers on the one side, and biological problems (he spent several years at the Institut Curie in Paris) on the other side. Within this subgroup Reza was working on a coarse grained model of DNA.

Although I was not directly involved in Reza's every day work, we had many discussions over the last years when it came to the details of a model, and I got a clear view on his role within this very active group.

The long-term goal is to understand the dynamic response of DNA to mechanical forces as they are exerted by binding enzymes. The first step is to create a hierarchy of DNA models on different length scales which are linked by a systematic coarse-graining procedure. In a second step we want to use this model for a systematic study of the

dynamic response of DNA to forces which are large enough to alter the local structure. This is a very challenging problem and complementary paths have to be followed which are somewhat different from what one typically does in systematic coarse-graining for most synthetic polymers. The team which started to look at this problem (R. Everaers as a senior scientist, and M. R. Ejtehadi as a postdoc) together with the overall research experience of the group turned out to be collaborating very well. Ralf Everaers' main experience was in continuum elastic worm like chain models and its application to biophysical problems while R. Ejtehadi had worked on toy models of proteins. The first crucial question which took some time to settle was to select the length scale where they were going to start modeling the molecule. To employ all atom models for the anticipated questions, as they are frequently used in computer simulations of molecular systems, certainly was not possible. Similarly, the typical semiflexible polymer models quite often employed in the theory of DNA are also not applicable. Weighing all the available information they decided to develop a method where parts of the DNA such as the bases, sugars and phosphates are treated as rigid bodies with simplified effective interactions, compared to atomistic simulations. As a consequence the corresponding potentials can be more complicated than those between point particles in standard simulation procedures. For example the van der Waals and excluded volume interactions between disc-like bases cannot be represented by simple 6-12 Lennard-Jones potentials. Similarly, chemical bonds reduce the relative motion of rigid entities such as sugar and base to rotations around non-centro-symmetric axis, a situation far from the behavior of two point particles connected by a harmonic spring. Taking this into account and keeping in mind that the simulation code had to be rather efficient in order to be able to run many systems for long enough times, it is clear that new simulation programs had to be written from scratch.

Based on such general concepts Reza developed a new object oriented C++ code which performs Monte Carlo Simulations of rigid bodies allowing for a fairly wide choice of generalized connectivities. With respect to non-bonded interactions between anisotropic bodies he developed a physically motivated simplification of the Gay-Berne potential which is often employed in liquid crystal simulations. At this point his careful and systematic manner of working out, implementing and testing details turned out to be important for the success of the project. He did this very independently and withstood many temptations to take a shortcut in such a highly competitive field. The result is a basic model and algorithm which is a very promising work horse for the next few years.

All this hard tedious work, in a sense, suppressed his productivity somewhat so that there are not that many papers which came out so far from his working time in Mainz. Right now he, together with a former student of the group (Boris Mergell), has produced a number of interesting results which are just published.

All together Reza is a pleasant and skillful collaborator who is truly motivated by biophysical problems. He was appreciated in the group as a scientist as well as a person.

Sincerely,

Kurt Kremer