

Dr Mohammad Reza Ejtehadi
Department of Physics and Astronomy
University of British Columbia
6224 Agricultural Road,
Vancouver, BC V6T 1Z1, Canada
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Biocomplexity Faculty Search committee,
c/o Prof. Rob de Ruyter van Steveninck,
Biocomplexity Institute,
Indiana University,

Subject: Job Application

Dear Faculty Search Committee,

Please find enclosed documents for your Assistant Professor position.

Here there is a list of the people, who can judge my abilities and works quality. I have arranged that you receive letters of reference from whose has been checked mark.

- Prof. Steven S Plotkin
University of British Columbia
Department of Physics and astronomy
6224 Agricultural Rd., Vancouver, B.C., V6T 1Z1, Canada
Phone: (604)822- 8813
Fax: (604)822-5324
email: steve@physics.ubc.ca

- Prof. Birger Bergeron
University of British Columbia
Department of Physics and astronomy
6224 Agricultural Rd.,
Vancouver, B.C., V6T 1Z1, Canada
Phone: (604)822-3853
Fax: (604)822-5324
email: birger@physics.ubc.ca

- Prof. Dr. Kurt Kremer
Max-Planck Institut für Polymerforschung
Ackermannweg 10
D - 55128 Mainz
Germany
Phone: +49 (0)6131 379 140
FAX: +49 (0)6131 379 340
Email: kremer@mpip-mainz.mpg.de

- Dr. Ralf Everaers
Max-Planck-Institut für Physik komplexer Systeme
Nöthnitzerstr. 38
01187 Dresden
Germany
Phone: +49 (0) 351 871 1206
fax : +49 (0) 351 871 1299
email : everaers@mpipks-dresden.mpg.de
- Prof. Hue Sun Chan
Department of Biochemistry
University of Toronto
1 King's College Circle
Medical Sciences Building
Toronto, Ontario M5S 1A8
Tel: 416-978-2697
email: chan@arrhenius.med.utoronto.ca
- Prof. Shahin Rouhani
Department of Physics
Sharif University of Technology
Tehran, Iran.
Tel. No.: +98-21-6164506
fax: +98-21-6005410
email: rouhani@ipm.ir
- Dr. Richard Goldstein
Division of Mathematical Biology
National Institute for Medical Research
The Ridgeway
Mill Hill, London, NW7 1AA, UK
Phone: +44 (0)20 8816 2293
Fax: +44 (0)20 8816 2460
e-mail: richard.goldstein@nimr.mrc.ac.uk

Sincerely yours,

Dr. Mohammad Reza Ejtehad

Research Plan

Mohammad Reza Ejtehadi

Personally as a physicist I am interested to study complex systems. The complexity inside these problems makes them interesting for me as like as a puzzle. During my PhD study and the years after I have worked on physics of soft condensed matter, and most of my works have been focused on physics of biological macromolecules. In these theoretical and mostly computer based studies we have looked on statistical, static and dynamical properties of proteins and DNA molecule. By the way, I would like to be in contact with other researchers in other interdisciplinary fields, and possibly collaborate with them, both theorists and experimentalists.

When I was working in my country, Iran, as an assistance professor (I leave there to join Max-Planck institute for polymer research in Germany as a post doctoral fellow, see CV), I had organized a small research group of undergraduate students. Most of the papers in my publication list which Iran is mentioned in their address are output of this group. Between five students working in my group, three of them have won the national prize for the best undergraduate study of the years in three years. Now all of them are nearly finishing their PhD programs in different universities around the world. One in MIT (USA), one in USC (USA), one in SFU (Canada), one in SISSA (Italy) and one in SUT (Iran). I hope in my new position I use my experience in working with undergrads and involving them to research projects in high standard level.

In the following I will explain some possible projects which I am interested to deal with them and I believe I have proper tools and enough experience to do them.

Possible research projects

Design and statical properties of proteins

1. After introducing the designability as a parameter which shows the attitude of the proteins to fold in a given structure [1], there are some evidences suggesting the solvation potential (equivalently additive potential [2, 3]) has most dominant effect on designability of lattice model proteins [4]. Some thing one can look is the importance of additive potential (solvation) in design of real proteins. A work in this direction is under progress. Further studies are possible.
2. In the pair contact models the structural information can be coded in a pair contact matrix. The compactness of native states of proteins which is a consequence of hydrophobicity forces, suggests that only a subset of these contact matrices can represent a designable structure [5]. In the case of additive potential the relevant structural information can be reduced more and it can be coded in a vector, named contact vector [6, 7]. The statistical properties of reduced space of contact matrices and contact vectors

as well as the structural properties of potentially independent designable proteins [8] can clarify some features of the design process.

3. Some recent experiments have shown a circular permutation stability in some proteins [9, 10, 11]. In the best of my knowledge nobody has studied the correlation between permutation symmetry and designability.

Mechanical properties of single molecules (DNA, RNA and proteins)

1. Advances in manipulation techniques of biopolymers allow the experimentalist to study and visualize the motion of individual single molecules such as DNA, RNA, actin and microtubules under the influence of thermal noise, solvent flows and external forces. In a recent work we have tried to understand the response of DNA molecules to external forces on different time and length scales at different temperatures [12]. This work is a Monte-Carlo based simulation study. The model is a generic model and can be applied to different macromolecules and even membranes [13]. The code which I have prepared to simulate the molecules is a C++ object oriented code with the flexibility to use for different molecules with different geometries. I hope to use this code to study dynamical properties of different types of macromolecules like RNA and proteins under influence of thermal noise and external force. Moreover, I hope to do some simulation on DNA with considering more details in molecule geometry. I believe there are lots of questions which we are able to investigate then using the model.
2. In DNA work mentioned above, we have introduced a new potential between ellipsoidal coarse grained objects [14]. However we have shown that our new potential is more accurate in estimating the Leonard-Jones potential between these extended objects than putative Gay-Berne potential, I think some works are necessary to popularize the new potential. In this direction, I would like ,
 - to parametrize the new potential for biological molecules,
 - to calculate forces and torques corresponding to this potential to prepare a molecular dynamics simulation code using the potential,
 - and to apply the new potential in a completely different problem, for example a liquid crystal simulation.

I am pretty sure some people working in “Max-Planck institute for polymer research” in Mainz, Germany, and “Max-Planck Institute for the physics of complex systems” in Dresden, Germany, would be interested to collaborate in these projects

Protein folding

Moreover, just now I am working on some problems to study mechanism of protein folding. I hope to continue to work in such problems in future.

References

- [1] H. Li, R. Helling, C. Tang, and N. Wingreen. Emergence of preferred structures in a simple model of protein folding. *Science*, 273, 1996.
- [2] M. R. Ejtehadi, N. Hamedani, H. Seyed-Allaei, V. Shahrezaei, and M. Yahyanejad. Stability of preferable structures for a hydrophobic-polar model of protein folding. *Phys. Rev. E*, 57, 1998.
- [3] N. E. G. Buchler and R. A. Goldstein. Surveying determinants of protein structure designability across different energy models and amino-acid alphabets: A consensus. *J. Chem. Phys.*, 112, 2000.
- [4] V. Shahrezaei and M. R. Ejtehadi. Geometry selects highly designable structures. *J. Chem. Phys.*, 113, 2000.
- [5] V. Shahrezaei, N. Hamedani, and M. R. Ejtehadi. Protein ground state candidates in a simple model: An enumeration study. *Phys. Rev. E*, 60, 1999.
- [6] M. R. Ejtehadi, N. Hamedani, H. Seyed-Allaei, V. Shahrezaei, and M. Yahyanejad. Highly designable protein structures and inter-monomer interactions. *J. Phys. A-Math. Gen.*, 31, 1998.
- [7] A. Kabakcioglu, I. Kanter, M. Vendruscolo, and E. Domany. Statistical properties of contact vectors. *Phys. Rev. E*, 65, 2002.
- [8] M. R. Ejtehadi, N. Hamedani, and V. Shahrezaei. Geometrically reduced number of protein ground state candidates. *Phys. Rev. Lett.*, 82, 1999.
- [9] M. Lindberg, J. Tangrot, and M. Oliveberg. Complete change of the protein folding transition state upon circular permutation. *Nat. Struct. Biol.*, 9, 2002.
- [10] S. Uliel, A. Fliess, and R. Unger. Naturally occurring circular permutations in proteins. *Protein Eng.*, 14, 2001.
- [11] J. Hennecke, P. Sebbel, and R. Glockshuber. Random circular permutation of DsbA reveals segments that are essential for protein folding and stability. *J. Mol. Biol.*, 286, 1999.
- [12] B. Mergell, M. R. Ejtehadi, and R. Everaers. Modeling DNA structure, elasticity, and deformations at the base-pair level. *Phys. Rev. E*, 68, 2003.

- [13] M. R. Ejtehadi and R. Everaers. Rigid-body formalism for simulating macromolecules. *Comput. Phys. Commun.*, 147, 2002.
- [14] R. Everaers and M. R. Ejtehadi. Interaction potentials for soft and hard ellipsoids. *Phys. Rev. E*, 67, 2003.

Statement of teaching

Mohammad Reza Ejtehadi

In very simple words I love teaching. From the time I have started my academic education I have taught in parallel. I have years of experience of teaching both in undergraduate and Physics Olympiad courses. I had this opportunity to teach in some classes filled by highly talent students. I believe teaching helps me to learn twice. Making a good communication with students is my goal in my classes. Nothing is more enjoyable for a teacher to see most of the students are following him. I believe as a researcher I should spend some time in teaching. It is an exercise for researcher's brain as like as the physical exercises for his body.

I think I would enjoy teaching both graduate and undergraduate courses. Both conceptual courses as like as Quantum Mechanics and Thermodynamics and advance courses like critical phenomena. I would like to incorporate activities into my classes which would prepare my students for research, such as computer programming.