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Joan and Sanford I. Weill
Medical College and
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Sergei Yu. Noskov, Ph.D.
Department of Physiology and Biophysics
1300 York Avenue, NY, NY 10021
Tel.: 212-746-4237; Fax: 212-746-4843
E-mail: syn2001@med.cornell.edu

To: Prof. Rob de Ruyter van Steveninck,
Biocomplexity Faculty Search Committee,
Department of Physics,
Indiana University, Swain Hall West 117,
Bloomington IN, 47405-7105

Dear Professor Rob de Ruyter van Steveninck,,

I am writing to apply for the position of assistant professor in computational structural biology. My research experience in the areas of biomolecular simulation, statistical mechanics and quantum chemistry have provided me with the background necessary to successfully assume the position you have described.

My scientific training encompasses several areas that fall under the heading of computational biology. My master's work focused on spectroscopic and quantum mechanical studies of hydrolysis mechanisms in bioorganic systems. This combination of interests defined my choice for a doctoral work at the Institute of Solution Chemistry of the Russian Academy of Sciences and the Institute of Theoretical Chemistry at Innsbruck University as Austrian Government fellow (OëAD fellowship). I was aimed to understand hydrophobic effects in complex systems and to develop new algorithms for molecular dynamics simulations, which provided a powerful instrument for studies of biomolecular dynamics at the atomic level. A growing interest in the simulation of proteins led me to join the Computational Biophysics Group of *Carmay Lim* at the Institute of BioMedical Sciences, Academia Sinica for my post-doctoral research. Major results of our efforts in understanding protein-ligand interactions were published in *Biophysical Journal*, *Nucleic Acids Research* and *Journal of Physical Chemistry B*.

Although I obtained expertise in the theoretical studies of protein-ligand interactions while working at the IBMS, I was interested in the understanding of the ways in which ions are trafficking to the cell. In 2002 I joined the group of Professor *Benoît Roux* at the Weill Medical College of Cornell University to work on the molecular origins of selectivity in ion channels. The importance of this work was recognized by the acceptance of our results for publication to *Nature* and *Biophysical Journal*. As noted in my curriculum vitae, I worked as a method developer for *CHARMM* program package to include account for an induced atomic polarization into modern biomolecular simulations. Results of our scientific efforts on the modeling of induced polarization in condensed phase and protein simulations will appear in the special issue of *Journal of Physical Chemistry B*.

I have enclosed a copy of my curriculum vitae, research plan, teaching statements and list of my scientific references.

I look forward to hearing from you.

Sincerely,



Sergei Yu. Noskov

Department of Physiology and Biophysics,
Weill Medical College of Cornell University

CURRICULUM VITAE

Sergei Yu. Noskov, Dr.Phil.

PROFESSIONAL ADDRESS:

Department of Physiology and Biophysics
Weill Medical College of Cornell University
Departments of Physiology and Biophysics
1300 York Avenue, New York, NY 10021
Phone: (212) 746-6018
Fax: (212) 746-4843
E-mail: syn2001@med.cornell.edu

EDUCATION:

POSTDOCTORAL TRAINING:

- 2002- Cornell University, Well Medical College, Department of Physiology and Biophysics, New York, New York, U.S.A. **Postdoctoral Fellow** with Prof. Benoît Roux. Research into biological channel function and polarizable force field development.
- 1999-2002 Institute of Biomedical Sciences, Academia Sinica, Computational Biophysics Group, Taiwan, Taipei. **Academia Sinica Postdoctoral Fellow** with Prof. Carmay Lim. Research in theoretical studies of protein-ligand binding and molecular dynamics of mutation effects on P53-DNA recognition.

POST-GRADUATE EDUCATION:

- 1996- 1999 Institute of Solution Chemistry, Russian Academy of Sciences (ISC RAS), Russia; Institute of General, Inorganic and Theoretical Chemistry, University of Innsbruck, Innsbruck, Austria. **Doctor of Philosophy** (Physical Chemistry) in Statistical Mechanics under supervision: Prof. Kolker A.M. (ISC RAS, Russia), Prof. Kiselev M.G. (ISC RAS, Russia) and Professor Dr. Dr.h.c. Bernd M. Rode (Austria).
Thesis Title: "The influence of collective effects on the selective ion solvation in water-alcohol-electrolyte systems. Molecular dynamics simulation."
- 1995- 1996 Department of Physical Chemistry, Ivanovo State University, Ivanovo, Russia. **Master of Science** (Physical Chemistry). Honors thesis in quantum chemistry and molecular spectroscopy (IR, UV and electron diffraction methods).

UNDERGRADUATE EDUCATION:

- 1991- 1995 Faculty of Chemical Biology, Ivanovo State University, Ivanovo, Russia. **Bachelor of Science:** Major: Chemistry. Minor: Biology; *Diploma cum Laude*.

SHORT-TERM APPOINTMENTS

1999 2004	Institute of Solution Chemistry, Russian Academy of Sciences, Department of Molecular Modeling/Theoretical Chemistry Core.	Junior Research Officer (1999-2001), Research Officer (2001-2004). Part-time appointment with ISC RAS. Co-advising of graduate students (3 students on the program in theoretical chemical biology (2001-2004) and teaching at a summer school of RAS. MD studies of hydrophobic hydration in mixed solvents.
2002	Royal Institute of Technology (KTH), Department of Physical Chemistry, Stockholm, Sweden	Visiting scientist (EU Research Fellow). <i>Ab-initio</i> and MD of Dnase cleavage mechanisms with Prof. Tore Brinck.
1996-1999	Department of Theoretical Chemistry, Highest Chemical College of Russian Academy of Sciences.	Teaching assistant , Lecturer in statistical mechanics and molecular simulations.
1993-1996	Ivanovo State University, Department of Physical Chemistry	Research assistant: IR, UV, Electron Diffraction and QM studies with Prof. Ivanov S.N.
1992,1993	National Child Development Center "Orlyonok", Tuapse, Russia	Camp counselor/tutor , Participant of special program of Russian Government in chemical education.

HONORS and AWARDS:

2004	American Epilepsy Foundation Postdoctoral Fellowship. (40.000 per year at Cornell University, AEF is part of Center of Disease Control, which supports research in neurosciences, structural biology and medicine of neurological diseases.)
2001-02	European Union (INTAS Foundations) Research Fellowship for Young Researchers. (9,000 per year at ISC RAS)
1999-02	Academia Sinica Post-Doctoral Fellowship. (Awarded to only top 5% candidates, 46.000 for 2 years at Academia Sinica)
1999-02	Russian Foundation for Basic Research , Team Grant, Grant role: Researcher (Highly competitive research grant from Russian Government for establishing of a new research in chemical biology and promoting of international scientific collaboration.)
1997-98	Austrian Government (OëAD) Doctoral Fellowship for international students. (10.000 per year. One of the most prestigious research fellowships in Austria).
1996-99	Russian Foundation for Basic Research , Team Grant, Grant role: Graduate Student at Department of Theoretical Chemistry and Molecular Modeling, ISC, RAS.
1993	Special Diploma of Russian Government (Ministry of Education) for participation in a program for chemical education at Russian National Center "Orlyonok", Tuapse, Russia.

LIST OF PUBLICATIONS:

1. Noskov SY, Berneche S, Roux, B: Control of ion selectivity in potassium channels by electrostatic and dynamic properties of coordinating ligands. *Nature*, 2004, vol. 431, p.830-834
2. Noskov S.Y., Lamoureux G., Roux B. " Microscopic picture of hydrophobic hydration in water-ethanol mixtures from simulation with new polarizable force-field". *J. Phys. Chem.B*, 2004, in press (invited paper)
3. Noskov SY, Kiselev M.G., Kolker A.M. Role of buried interface water in protein association. *Biofizika*, 2004, in press.

4. Noskov SY, Im W, Roux B. Ion Permeation through the alpha-hemolysin Channel: Theoretical Studies Based on Brownian Dynamics and Poisson-Nernst-Planck Electrodiffusion Theory. *Biophys. J.*, 2004, vol.87, p. 2299-2309
5. Noskov SY, Wright JD, Lim C., Long-Range Effects of Mutating R248 to Q/W in the p53 Core Domain *J. Phys. Chem. B*, 2002, 106; 13047-13057
6. Wright J.D., Noskov S.Y., Lim C. Factors governing loss and rescue of DNA binding upon single and double mutations at P53 core domain. *Nucleic Acids Research*, 2002, 30; 1563-1574
7. Kiselev M.G., Noskov S.Y., Puhovski Y.P., Kerdcharoen T., Hannongbua S. Study of hydrophobic hydration in super-critical methanol-water mixtures. *J. Mol. Graph. Model.*, 2001, 19; 412-416
8. Noskov S.Y., Lim C. Free energy decomposition of protein-protein interaction. *Biophys. J.*, 2001, 81;737-750
9. Noskov S.Y, Kiselev M.G, Kolker A.M, Rode B.M. Structure of methanol-methanol associates at dilute methanol-water mixtures from molecular dynamics simulation. *J. Mol. Liq.*, 2001, 91; 157-165
10. Noskov S.Y, Kiselev M.G, Kolker A.M Structural aspects of NaCl solvation in water-methanol mixtures from molecular dynamics simulation. *Rus. J. Phys. Chem.*, 2001, 75; 380-386
11. Petrov VM, Petrova VN, Kislov VV, Ivanov SN, Noskov SY, Krasnov AV, Bylova ZM Electron diffraction and quantum chemical study of the molecular structure of para-methylbenzenesulfonyl fluoride and para-methylbenzenesulfonyl bromide. *J. Struct. Chem.*, 2000, 41; 939-945
12. Kislov VV, Petrov VM, Noskov SY, Petrova VN, Ivanov SN Molecular structure of p-methyl benzene sulphonyl halides and benzene sulphonyl chloride from quantum-mechanical calculations and gas-phase electron diffraction *Int. J. Chemistry.*, 1999, 2; 9
13. Petrov V.M, Petrova V.N, Kislov V.V, Ivanov S.N, Girichev G.V, Noskov S.Y, Krasnov A.V, Electron diffraction and quantum chemical study of the molecular structure of 4-methylbenzene sulfochloride. *J. Struct. Chem*, 1999, 40 ; 533-540
14. Noskov, S.Y., Kiselev, M.G. and A.M.Kolker. Many body effects in simple liquids. *Int. J. Chemistry*, (1998) 1; 9
15. Noskov S.Y., Kiselev M.G., Kolker A.M., Molecular dynamic study of the anomalous behavior of heat capacity in a methanol-water mixture. *J. Struct. Chem.*, 1999, 40; 253-261
16. Kislov V.V., Ivanov S.N., Noskov S.Y., Extreme modification of activated parameters of para-toluenesulfobromide hydrolysis in water dioxane. Interrelation with the solvent structure. *Rus. J. Gen. Chem.*, 1997, 67;1330-1337

Monograph's chapter:

- M.G. Kiselev, S.Y. Noskov, D.V. Ivlev, S.P. Krishtal, Y.P. Puhovski, A.V. Borodin, A.M. Kolker "Macromolecular association in liquid media: Theory meets experiment" in *Advances in Solution Chemistry*, Moscow, "Nauka", 2005, *in press*

Submitted to Journal:

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- Noskov S.Y., Lim C. "Role of interfacial water in a weak protein association: CD2-CD58 binding", *Proteins*, 2004 submitted

Recent conference contribution:

- Noskov, SY, Berneche S., Roux, B. "Molecular Origin of Ion Selectivity in K⁺ channels", Gordon Research Conference "Ion Channels-2004"
- Noskov SY, Lamoureux G., Roux, B. "Modeling of hydrophobic effects with a polarizable force field", Gordon Research Conference "Water and Aqueous Solutions -2004"
- Noskov SY, Berneche S, Roux B" The microscopic origin of ion selectivity in potassium channels". *Biophys. J.* 86 (1): 351A-352A Part 2 Suppl., 2004
- Anisimov V.M., Vorobyov I.V., Lamoureux G., Noskov S., Roux B., MacKerell A.D.
- CHARMM all-atom polarizable force field parameter development for nucleic acids *Biophysical J.*, 86 (1): 415A-415A Part 2 Suppl., 2004
- Noskov S.Y., Lim C., Kiselev M.G., Kolker A.M. "Contribution of buried water to stability of protein-ligand complexes". Invited Speaker at 17-th International Congress on Chemical Thermodynamics, Russia, 2002
- Noskov S.Y., Brinck, T. "Mechanism of DNA cleavage by Dnase E7. Quantum-mechanical studies" V.A. Fock International School on Quantum Chemistry, 2003

Projects under working progress:

- QM/MM studies of ion hydration in K⁺ channel cavity at different temperatures
- BD simulations of ion conductance through different iso-forms of KcsA (thermodynamics of gating).
- GCMC/BD studies of ion conductions in MscS channel
- Polarizable force-field development.

Reviewer for the *Biophysical Journal* since 2004 (section Bio-Molecular Modelling, Ion Channels)