Dr. Artëm Masunov
Postdoctoral Research Associate
Los Alamos National Laboratory
Theoretical Chemistry and Molecular Physics
T-12, MS B268
Los Alamos, New Mexico 87545
(505) 665-2635 / Fax (505) 665-3909
Email: amasunov@t12.lanl.gov

November 21, 2004

Biocomplexity 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 Search Committee Chair,
I would like to apply for Assistant Professor position in Computational Biochemistry at Indiana University.

My area of expertise includes computational chemistry, biophysics, and materials science. I have had successful experiences in both teaching and research. Apart form the six years of teaching assistantship, I had six years of independent undergraduate teaching experience as a junior faculty. I mentored thesis projects of three undergraduate students and supervised summer internships of two graduate students. Each of them resulted in publications. I have worked in US and European Universities and at present am working at Los Alamos National Laboratory. I was pursuing computational research in the areas of crystal engineering, molecular recognition and self-assembly by means of hydrogen bonding and other intermolecular interactions, solvent effects, molecular dynamics of solutions and proteins, ligand/receptor binding free energy, electronic structure of solids and nonlinear optical materials. Furthermore, I served as a reviewer for *Phys. Rev. B, J. Phys. Chem*., *J. Am. Chem. Soc., Macromol. Theor. Sim.* and *Encyclopedia of Polymer Sci*.

I also had successful experience in grantsmanship, examples of my research proposal writing include the study of solvent effects on two-photon absorbing properties (for LANL-UCSB Collaborative Research Program), targeted drug delivery for cancer treatment (for Laboratory Directed Research and Development program of LANL), and computational design of nonlinear optical materials (for DOD DARPA program). My proposal "Computationally guided control of nanomaterial synthesis: carbon nanotube growth catalyzed by metal nanoparticles" was funded for FY2005 ($55,000) under LANL-UC CARE program. I closely collaborated with experimentalists on most of my research projects.

Please find enclosed my curriculum vitae and statement of my research interests. My proposed projects involve nanofibers, nanotubes, nanocrystals, enzymes, photoactive proteins; applications include nonlinear optical bioimaging, photodynamic therapy, rational drug design and neurodegenerative disease treatment. Thank you for considering me as a candidate.

Sincerely yours, Artëm Masunov

ARTËM MASUNOV

MS B268, T-12, LANL, Los Alamos, NM 87545; http://www.t12.lanl.gov/home/amasunov
Home: (917) 251-5536; Office: (505) 665-2635; E-mail: amasunov@t12.lanl.gov

Education:

2000 – Ph.D., Chemistry, *The City University of New York, NY*. Thesis: "Molecular and crystal orbital studies of organic crystal formation". Mentor: Prof. J.J. Dannenberg
1988 – Diploma (BS/MS), Chemistry, *Moscow State University, Russia*. Thesis: "Interpretation of experimental electron density distribution in crystals". Mentor: Prof. P.M. Zorkii

Areas of Expertise:

Computational, quantum, and theoretical chemistry, biophysics and materials science. *Methods*: density functional theory, multiconfigurational methods, molecular dynamics, orbital models of intermolecular interactions, solvation models. *Applications*: molecular crystals, proteins, nanocrystals and nanomaterials, excited states, organic two-photon absorbing materials.

Research Experience:

2002-present: Postdoctoral Research Associate, *Theoretical Chemistry and Molecular Physics group, Los Alamos National Laboratory, NM* (with Dr. S.Tretiak)

- Interfaced Gaussian 98 with CEO suite of programs to calculate Two-Photon Absorption Cross-Section at Time-Dependent Density Functional Theory level; modified code can be used for photonics applications
- Found that at both one- and two-photon absorption transition energies are accurately reproduced by Time-Dependent DFT method (error is 4% at TD-B3LYP/6-31G level for a set of 24 bis(styril)benzene derivatives); two-photon absorption cross-sections are among the best theoretical predictions as well.
- Modified Kohn-Sham formalism of Density Functional Theory to describe strongly correlated systems

2002-2003: Part-time Research Associate, *Polymer Institute, University of California at Santa Barbara, CA* (with Prof. G.Bazan)

- Predicted two-photon absorption spectra of organic chromophores, and compared them to the experiment
- Studied solvent effects on absorption and emission spectra of [2.2]paracyclophane derivatives

2000-2002: Postdoctoral Fellow, *Computational Biophysics group, City College of New York, The City University of New York, NY* (with Prof. T.Lazaridis)

- Proposed a novel microscopic implicit solvation model, based on average solvent charge distribution.
- Tabulated potentials of the mean force for ionizable amino acid side chains in aqueous solution obtained in explicit MD simulations using Umbrella/WHAM technique for future solvation model development
- Augmented MD simulations of binding free energy of biotin with avidin/streptavidin by quantum mechanical calculations of the binding site

1994-2000: Thesis Research, *The Graduate School, The City University of New York, NY* (with Prof. J.J.Dannenberg)

- Estimated sublimation enthalpy and relative crystal polymorph stability for urea and thiourea at *ab initio* level
- Revealed the critical importance of cooperative effects in hydrogen bonding on crystal structure
- Developed subminimal floating-gaussian basis set for QM/MM studies of intermolecular interactions

1988-1994: Scientist/Jr. Scientist, *Organic Crystal Chemistry Lab., Chemistry Faculty, Moscow State University, Moscow, Russia* (with Prof. P.M.Zorkii)

- Studied the origin of variations in bioactivity of 6-methyluracile samples. On the basis of analytical comparison of analogous crystal structures predicted the structure of the second polymorph modification. Variations in bioactivity linked to crystal structures through the agglomeration in aqueous solutions
- Developed real space structural model for electric conductivity in crystals applicable to design new high-T_c superconductors and based on analysis of potential energy function in local symmetry coordinates.
- Reviewed and classified existing methods of electron density distribution analysis and developed a new method allowed to compare continuous 3D-distribution of the same topology but different geometry, which is applicable to broader range of problems
- Analyzed geometric parameters of Cl...Cl and M...Nu (M=3d-transition metal, Nu=N,O) intermolecular contacts in crystal structures. Statistically meaningful preferences were found to support hypothesis of partially covalent nature of this contacts.
- Conducted systematization of para-substituted biphenyl crystal strictures, established common features revealing the importance of CH...π, OH...O, CN...Br, Br...Br, Cl...Cl and HS...SH intermolecular interactions for crystal structure formation.
- Created and developed integrated software package for geometrical analysis of molecular crystals.

Teaching Experience:

Summer 2003,2004: Research supervision and mentoring of two graduate students (*Los Alamls Natl. Lab.)*
Spring 1999-Spring 2000: General Chemistry Laboratory: Graduate instructor (*Hunter College)*
Fall 1997-Fall 1998: Physical Chemistry Laboratory: Graduate instructor (*Hunter College)*
Fall 1995-Spring 1996: Organic Chemistry Laboratory: Graduate instructor (*Hunter College)*
Fall 1994-Spring 1995: General Chemistry Laboratory: Graduate instructor (*Hunter College)*
Fall 1992: Electronic models of Molecules and Solids: Lecturer (*Moscow State University)*
Fall 1991-Spring 1993: Supervised Diploma projects of three students (*Moscow State University)*
Fall 1990-Spring 1993: Crystallography: Substitute Lecturer (*Moscow State University)*
Fall 1988-Spring 1993: Symmetry in Molecules and Crystals: Instructor (*Moscow State University)*
1990-1993: Research and Diploma thesis supervision of three undergraduate students (*Moscow State University)*

Awards:

2004 – Research Grant "Computationally guided control of nanomaterial synthesis: carbon nanotube growth catalyzed by metal nanoparticles", *LANL-UCDavis Cooperative Agreement for Research and Education Program*
2003 – Outstanding Post Doctoral Poster Presentation in Chemistry, *Los Alamos National Laboratory, Los Alamos, NM*
1998 – Travel Award, *American Chemical Society, San Francisco, CA*
1997 – Travel Award, *American Crystallographic Association, St. Luis, MO*
1997 – Travel Award, *International Congress of Quantum Chemistry, Atlanta, GA*
1995 – Travel Award, *American Crystallographic Association, Montreal, Canada*
1995 – Travel Award, *International Union of Crystallography, La Plata, Argentina*
1994 – Junior Scientist Research Award, *American Crystallographic Assoc.*
1993 – Travel Award, *International Science Foundation, Beijing, China*
1993 – Travel Award, *International Union of Crystallography, Fuzhou, China*
1993 – Russian Scientist Research Award, *International Science Foundation*
1992 – Travel Award, *Swiss Crystallographic Association, Geneva, Switzerland*
1990 – Travel Award, *European Crystallographic Union, Enschede, The Netherlands*
1991 – Junior Scientist Research Award, *Chemistry Faculty, Moscow State University, Russia*
1981, 1982, 1983 – Winner of the National Student Olympiads in Chemistry, *USSR*

Invited talks:

2004 – Chemistry Division, Argonne National Lab, Argonne, IL
2004 – Chemistry Department, New Mexico Tech, Socorro, NM
2003 – Science Department, New Mexico Highlands University, Las Vegas, NM
2003 – Excited State Processes'03, Los Alamos, NM
2003 – Arizona Days'03, Arizona State University, Tucson, AZ
2002 – Merck Analytical Research Labs, Rahway, NJ
2001 – Theoretical Division, Los Alamos National Lab, Los Alamos, NM
2001 – School of Pharmacy, University of Kansas, Laurel, KS

Synergistic Activities:

1985-1987: Freshmen Career Adviser, *Chemistry Faculty, Moscow State University*
1998: Beta tester of *ChemOffice* for CambridgeSoft.
1998: Referee for the *Proceedings of the Symposium on Parallel Quantum Chemical Calculations, Spring 1997 ACS Natl. Meeting*
1999: Internet service reviewer for the *Journal of the Chemical Information and Computer Science*
2000-present: Referee for the *Journal of the American Chemical Society*
2004-present: Referee for the *Macromolecular Theory and Simulations*
2004-present: Referee for the *Journal of Physical Chemistry*
2004-present: Referee for the *Physical Reviews*
2004: Referee for the *Encyclopedia of Polymer Science, 3rd Edition*

Professional References:

1. Prof. J.J. Dannenberg, City University of New York - Hunter College and The Graduate School, 695 Park Ave., New York, NY 10021; tel:212-772-5343; fax:212-772-5332; jdannenberg@gc.cuny.edu; http://patsy.hunter.cuny.edu/FandS/JJD/dannenberg.html
2. Dr. Sergei Tretiak, Staff Member, Theoretical Division, Los Alamos National Laboratory, MS B268, Los Alamos, NM 87545; tel:505-667-8351; fax:505-665-3909; serg@lanl.gov; http://www.t12.lanl.gov/home/serg
3. Prof. Mikhail Yu. Antipin, D.Sc., Corresponding Member of The Russian Academy of Science, Laboratory Head, Director of X-Ray Structural Centre, A.N. Nesmeyanov Institute of Organoelement Compounds (INEOS), Russian Academy of Sciences, 28 Vavilov St., B-334, Moscow 119991, Russia; tel:7-095-135-9215; fax:505-454-3103; m_antipin@yahoo.com; http://www.ineos.ac.ru/~xray

Additional References:

4. Dr. Antonio Redondo, T-12 Group Leader, Theoretical Division, Los Alamos National Laboratory, MS B268, Los Alamos, NM 87545; tel:505-667-9738; fax:505-665-3909; redondo@lanl.gov; http://www.t12.lanl.gov/home/redondo
5. Prof. Anna Krylov, Department of Chemistry, SSC #409, University of Southern California, Los Angeles, CA 90089-0482; tel:213-740-4929; fax:213-740-3972; krylov@usc.edu; http://www-rcf.usc.edu/~krylov
6. Prof. Guillermo C. Bazan, Polymer Institute, University of California Santa Barbara, CA 93106; tel: (805)893-5538; bazan@chem.ucsb.edu; http://www.chem.ucsb.edu/~bazangroup
7. Prof. Themis Lazaridis, Computational Biophysics Lab, City College of New York, Convent Avenue at 138th St., New York, NY 10031; tel:212-650-8364; fax:212-650-6107; themis@sci.ccny.cuny.edu; http://www.sci.ccny.cuny.edu/~themis
8. Prof. Tatiana Polenova, Chemistry & Biochemistry, 245 Brown Lab, University of Delavare, Newark, DE 19716; tel:302-831-1968; fax:302-831-6335; tpolenov@chem.udel.edu; http://www.udel.edu/chem/polenova/polenova.html

Publications:

1. Masunov A. When density functional theory goes wrong and how to fix it: spin balanced unrestricted Kohn-Sham formalism. physics/0310106
2. Masunov A., Tretiak S., Hong, J., Bazan G.C. Theoretical study of the effects of solvent environment on photophysical properties and electronic structure of paracyclophane chromophores. *J. Chem. Phys.*, In preparation
3. Kobko N., Masunov A., Tretiak S. Calculations of the third-order non-linear response in push-pull chromophores with time-dependent density functional theory. *Chem. Phys. Lett.* 392(4-6): 444-451, 2004
4. Masunov A., Tretiak, S. Prediction of two photon absorption properties of organic chromophores using the time-dependent density functional theory. *J. Phys. Chem. B,* 108(3): 899-907, 2004
5. Toulokhonova I.S., Stringfellow T.C., Ivanov S.A., Masunov A., West R.A. Disilapentalene and a stable diradical from the reaction of a dilithiosilole with a dichlorocyclopropene. *J. Am. Chem. Soc.* 125(19): 5767-73, 2003
6. Masunov A., Lazaridis T. Potentials of mean force between ionizable amino acid side chains in water. *J. Am. Chem. Soc.* 125(7):1722-30, 2003
7. Mallik B., Masunov A., Lazaridis T. Distance and exposure dependent effective dielectric function. *J. Comput. Chem.* 23(11):1090-9, 2002
8. Lazaridis T., Masunov A., Gandolfo F. Contributions to the binding free energy of ligands to avidin and streptavidin. *Proteins* 47(2):194-208, 2002
9. Masunov A. ACD/I-Lab 4.5: An Internet service review. *J. Chem. Inf. Comp. Sci.* 41(4): 1093-95, 2001
10. Masunov A. Introduction to perturbation theory in quantum mechanics by Francisco M. Fernandez (University of La Plata, Argentina). CRC Press LLC: Boca Raton, FL. 2001. xii + 272 pp. $99.95. ISBN 0-8493-1877-7. *J. Am. Chem. Soc.* 123(26): 6464, 2001
11. Masunov A., Dannenberg J.J., Contreras R.H. C-H bond-shortening upon hydrogen bond formation: Influence of an electric field. *J. Phys. Chem. A.* 105(19): 4737-40, 2001
12. Masunov A., Molecular and crystal orbital studies of the organic crystal formation. PhD Thesis. City University of New York, 2000. http://www.t12.lanl.gov/home/amasunov/diss/phd.htm
13. Masunov A., Dannenberg J.J. Theoretical study of urea and thiourea. 2. Chains and ribbons. *J. Phys.Chem. B.* 104(4):806-10, 2000
14. Cardenas-Jiron G.I., Masunov A., Dannenberg J.J. Molecular orbital study of crystalline p-benzoquinone. *J. Phys. Chem.* 103(35):7042-6, 1999
15. Dannenberg J.J., Haskamp L., Masunov A. Are hydrogen bonds covalent or electrostatic? A molecular orbital comparison of molecules in electric fields and H-bonding environments. *J. Phys. Chem.* 103(35):7083-6, 1999
16. Masunov A., Dannenberg J.J. Theoretical study of urea. I. Monomers and dimers. *J.Phys. Chem.*103(1):178-184, 1999
17. Giribet C.G., Vizioli C.V., Deazua M.C.R., Contreras R.H., Dannenberg J.J., Masunov A. Proximity effects on nuclear spin-spin coupling constants. Part 2. The electric field effect on $_1$J(CH) couplings. *J. Chem. Soc.-Faraday Trans.* 92(17):3029-3033, 1996

18. Masunov A., Dannenberg JJ. A theoretical investigation of the C-H...O interaction between substituted phenylacetylenes and water. *Theochem-J. Mol. Struct.* 371:17-19, 1996
19. Vyboishchikov S.F., Masunov A.E. Topological properties of electron density in the H^- $+H_2CO$ reaction system. *Theochem-Journal of Molecular Structure.* 117:161-167, 1994
20. Vyboishchikov S.F., Masunov A.E., Streltsov V.A., Zorkii P.M., Tsirelson V.G. Topological analysis of electron density in a chlorine crystals. [Russian] *Zhurnal Fizicheskoi Khimii.* 68(11):2024-2028, 1994 [English Ed.] *Russ.J.Phys.Chem.* 68(11):1837-40, 1994
21. Gladkikh O.P., Masunov A.E., Leonidov N.B., Belsky V.K. Polymorphism of 6-methyluracil. *Int. Union Crystallogr., Crystallogr. Symp. (Correlations, Transformations, and Interactions in Organic Crystal Chemistry)* 7: 266-288, 1994
22. Masunov A.E., Gladkikh O.P., Zorkii P.M. Structure-relaxation mechanism of electrical conductivity of crystals. *Russ.J.Phys.Chem.* 67(7): 1275-1277, 1993
23. Leonidov N.B., Zorkii P.M., Masunov A.E., Gladkikh O.P., Belskii V.K., Dzyabchenko A.V., Ivanov S.A. Structure and biological nonequivalence of polymorphic forms of 6-methyluracil. *Russ. J. Phys. Chem.* 67, 2220-2223, 1993
24. Masunov A.E., Grichshenko S.I., Zorky P.M. Influence of specific intermolecular interactions on crystal structure. Uracil derivatives and analogs. *Russ. J. Phys. Chem.* 67(2): 201-217, 1993
25. Masunov A.E. Stereoelectronic model of the structure of layered crystals of binary dihalides. [Russian] *Koordinatsionnaya Khimiya.* 19(4):261-8, 1993 [English Ed.] *Russ.J.Coord.Chem.* 19(4):242-9, 1993
26. Panfilov T.N., Gladkikh O.P., Masunov A.E., Poraj-Koshits M.A. Steric shielding of the metal atom in complexonates by using the computer program TPSE. *Russ. J. Coord. Chem.* 19(1): 11-14, 1993
27. Masunov A.E., Zorky P.M. Donor-acceptor nature of specific nonbonded interactions of sulfur and halogen atoms. Influence on the molecular geometry and packing. *Russ. J. Struct. Chem.* 33(3): 423-435, 1992
28. Masunov A.E., Grichshenko S.I., Zorky P.M. Influence of specific intermolecular interactions on crystal structure. Para-substituted biphenyl derivatives. [Russian] *Zhurnal Fizicheskoi Khimii.* 66(1):46-59, 1992 [English Ed.] *Russ.J.Phys.Chem.* 66(1):23-30, 1992
29. Masunov A.E., Zorky P.M. Geometric characteristics of Halogen...Halogen intermolecular contacts in organic crystals [Russian] *Zhurnal Fizicheskoi Khimii.*66, 60-69, 1992 [Eng.Ed.] *Russ. J. Phys. Chem.* 66, 31-35, 1992
30. Zorky P.M., Masunov A.E. X-ray diffraction studies on electron density in organic crystals. [Russian] *Uspekhi Khimii.* 59(7): 1027-1051, 1990 [English Ed.] *Russian Chemical Reviews.* 59(7): 529-606, 1990
31. Masunov A.E., Zorky P.M. Quantitative comparison of continuous charge distributions in molecules. [Russian] *Vestnik Moskovskogo Universiteta. Ser.2; Khim.* 29(2):131-136, 1988