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**Theoretical Division**  
**Theoretical Chemistry and Molecular Physics**

Date: December 8, 2004

Dear Search Committee:

I am pleased to write this letter to recommend Dr. Artem Masunov for the faculty position at your University.

Dr. Masunov is a gifted and experienced scientist with broad theoretical background, creativity, and skills in the computational chemistry. He obtained masters level graduate education in chemistry at Moscow State University, subjectively the strongest research institution in Russia. After that Artem has been a junior faculty at Moscow State University for 6 years where he obtained diverse "hands on" research experience resulted in 10 publications in Russian peer-review journals. In 1994 he entered the graduate program in chemistry at the City University of New York with Prof. J. Dannenberg. In 2000-2002, Artem worked at CUNY as a postdoc gaining extensive experience in the applied theoretical chemistry. He joined my group at Los Alamos National Laboratory as a postdoc just over two years ago.

During his first year at Los Alamos, Dr. Masunov has been working on development of accurate computational approaches for prediction of nonlinear optical response in the organic electronic materials. A new methodology based on the quasiparticle representation of the time dependent density functional theory (TDDFT) has been proposed. This method allows efficient calculations of arbitrary second and third order nonlinear optical responses in the extended molecular systems. Artem extensively developed this novel technique and made an efficient computational implementation by interfacing commercial Gaussian program suite with the collective electronic oscillator (CEO) package. Furthermore, he did massive testing of the new method by computing one- (linear response) and two- (third-order response) photon absorption spectra in a series of donor-acceptor substituted conjugated molecules. Calculated excitation energies are found to be in excellent agreement with experiment for all excitation frequencies across the entire set of molecules with the mean error of about 4% for both one and two photon transition energies. This is a drastic improvement over the other computational methods where typical errors are about 20%. The evaluated two-photon absorption cross-sections agreed with experimental spectroscopy as well. The paper on this study has been published in the *J. Phys. Chem.* (January 2004).

Dr. Masunov excelled not only in the method-development but also in several practical applications of the computational chemistry to specific molecular systems by closely interacting with the synthetic group of Prof. G.C. Bazan at UCSB. During his second year at LANL, he conducted thorough investigations of dielectric medium effects on linear and nonlinear spectra of soluble chromophores in several solvents spanning the wide range of dielectric constants (from hexane to water). The results explain observed experimental solvatochromatic trends and elucidate the applicability of various theoretical solvent models to centrosymmetric solutes. One paper on this study has been submitted to *J. Chem. Phys.* and another one will be submitted shortly.

At Los Alamos, Dr. Masunov has shown himself as a broad researcher open for the discussions in very different areas. He is involved in various materials science programs at LANL ranging from molecular based quantum computing to electronic structure and spectroscopy of semiconductor nanocrystals. In every occasion he provides valuable expertise and advice to our colleagues working in experiment/theory/modeling. He was actively participating in several research proposals as PI and co-PI submitted to internal (e.g. LDRD) and external (e.g. DARPA) funding agencies. In particular, Dr. Masunov initiated collaboration with Prof. Ting at UC Davis which resulted in a funded proposal "Computationally guided control of nanomaterial synthesis: carbon nanotube growth catalyzed by metal nanoparticles" under LANL-UC Davis Cooperative Agreement for Research and Education Program (CARE).

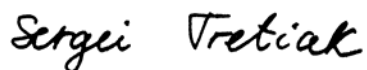
Artem has presented his research results on several National Meetings, local LANL conferences, and group seminars. His talks are clear and interesting for the audience. He won several awards for the best poster and the best postdoc talk. Dr. Masunov has also shown himself as an excellent mentor of graduate students by mentoring two summer students in 2003 and 2004, respectively. Both students were participant of undergraduate/graduate summer student program sponsored by Center for Nonlinear Studies at LANL. They have made substantial scientific progress resulted in peer-review publications (Chem. Phys. Lett (2004) and JACS (submitted)). I expect Artem to be a good lecturer and a teacher/mentor of students.

I have been delighted with Dr. Masunov's performance as a postdoc. He demonstrated the high level of maturity and identified himself as an independent researcher. Very little guidance was required from me to direct his research. I found him to be highly motivated, talented, creative and hardworking. In addition, his breadth is truly amazing. Artem has a good mathematical, physical and computational background. He is able for both method development and application work. On the personal side, he has a pleasant, polite and outgoing personality, which allows him to interact well with all of his colleagues. It was a pleasure working with him.

In his proposal Dr. Masunov outlines an excellent research program related to the theoretical modeling of diverse molecular systems and physical phenomena which demonstrates his wide-range expertise. This project and the scope of his interests are closely connected to current experiments. Artem will certainly fit into any chemistry/physics department and will strongly enhance and support development of physical chemistry/spectroscopy/materials science/nanotechnology programs.

In summary, Dr. Artem Masunov is a very capable researcher, and I recommend him to you most highly. Please feel free to contact me if you would need any additional information.

Sincerely,

The image shows a handwritten signature in black ink that reads "Sergei Tretiak". The signature is written in a cursive, slightly slanted style.

Sergei Tretiak, Ph.D.