

## Stanislav M. Avdoshenko, Age 29

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| CONTACT INFORMATION   | <p>Purdue University<br/>School of Materials Engineering<br/>West Lafayette, IN 47907-2045<br/>USA</p>  | <p>Cell:(765) 496-6350<br/>Fax :(765) 496-6026<br/>E-mail: savdoshe@purdue.edu<br/>WWW: Homepage</p> |
| OBJECTIVE             | Placement in a postdoctoral position doing research in theoretical materials science  |  |
| CITIZENSHIP           | Russia  |  |
| DATE OF BIRTH, PLACES | 19.03.83, Kaluga, Russia  |  |
| RESEARCH INTERESTS    | Molecular modeling, properties of complex and dynamic systems, advance theoretical algorithms, computing, electronic structure theory, response theory, biosystem behavior, education.  |  |
| EDUCATION             | <p><b>The Moscow State University</b>, Moscow, Russia</p> <p>Dr.rer.nat, Department of Chemistry, March 2009</p> <ul style="list-style-type: none"><li>• Thesis Topic: <i>Isomerism and its influence on the properties of the fluorinated carbon clusters</i></li><li>• Thesis Proposal: <i>Structure-property correlations</i></li><li>• Candidacy Exam: <i>Philosophy of science, Physical Chemistry</i></li><li>• Advisers: Professor Lev N. Sidorov and Dr. Ilay N. Ioffe</li><li>• Area of Study: Physical Chemistry, Theoretical chemistry</li></ul> <p>M.S. with honor, Department of Material science, January 2007</p> <ul style="list-style-type: none"><li>• Thesis Topic: <i>Theoretical and experimental study of structure and rearrangements of fullerene derivatives</i></li><li>• Thesis Proposal: <i>Dynamical processes in molecules</i></li><li>• Advisers: Professor Lev N. Sidorov and Dr. Ilya N. Ioffe</li><li>• Area of Study: Physical Chemistry</li></ul> |  |
| ACADEMIC APPOINTMENTS | <p><b>Postdoctoral Researcher</b><br/>Group Prof. Strachan<br/>Purdue University,<br/>School of Materials Engineering</p> <p><b>Postdoctoral Researcher</b><br/>Group Prof. Cuniberti<br/>Department of Material Science,<br/>Technical University Dresden</p>  | <p>2012 to present</p> <p>2009 to 2012</p>   |
| REFeree FOR JOURNALS  | <ul style="list-style-type: none"><li>• <i>Journal of Physical Chemistry A, B, C</i></li><li>• <i>Journal Phys. Chem. Chem. Phys.</i></li><li>• <i>Physical Review B</i></li></ul>  |  |

## AWARDS

- Erasmus Mundus program, DAAD 2009
- Moscow grants for perspective students and scientist, 2007
- Leonhard-Euler-Scholarship, DAAD 2006
- Moscow State University grants for students and young scientists, 2006

## TEACHING EXPERIENCE

**The Moscow State University**, Department of Chemistry  
**TU Dresden**, Materials Science department

### *Teaching Assistant*

**September 2007 to March 2008**

- Instructor for Physical Chemistry and Statistical physics.
  - Sample student evaluations available upon request.
  - Responsible for 1/2 hour lecture and tasks explanation for 1/2 hour where senior undergraduate students work on the physical and statistical problems.
  - Oral examination and colloquiums.

### • Molecular modeling courses

**September 2009 to March 2010**

- Sample student evaluations available upon request.
- Responsible for supervision of undergraduate students learn how to use molecular programming codes to study properties of the matter at different scales.
- Developed supplementary courses and problem design Material and problem sheets available upon request.

## TECHNICAL SKILLS

### *Theoretical methods*

- Quantum chemical (mostly DFT) computations of structure, properties, IR, optical, and X-ray spectra, reaction pathways, properties of continuous systems, band structure analysis, etc. Computation of X-ray spectra by means of multiple scattering formalism. Non-equilibrium Green function computations of transport properties.
- Software and packages PRIRODA (DFT code), GAMESS (general quantum chemistry package), CRYSTAL98-03/VASP (continuous systems), DFTBg+ (continuous systems, Green function formalism), FEFF8 (multiple scattering process), CP2k/CPMD (modern MD code ab-initio/ QMMM/classical), AMBER10 (classical and semi-empirical MD), NAMD2(classical MD), VMD scripting

### *Experimental techniques*

- Mass-spectrometry (Electrospray, MALDI), electron and atomic force microscopy, certain experience in NEXAFS, photoelectron spectroscopy (X-ray and UV), ion beam and other deposition techniques.

### *Experimental practice*

- 3 months work (diploma practice): Kurchatov Synchrotron Radiation source, Moscow Russia, soft and hard X-ray station and NEXAFS/EXAFS spectra simulation for self assembled mono-layers and for biomolecules (the real time on the NEXAFS station around 3 weeks).
- 2 weeks work (Karlsruhe University, Institute of Physical Chemistry): MS-ESI-PES (photo-electron spectroscopy) tandem analysis.
- 1 months work (DAAD practice, Bundesanstalt für Materialforschung und -prüfung): BESSY

- synchrotron radiation source, soft X-ray station (the real time on the station around 1 week).
- Long practices in MALDI/ESI technique.

Programming: C, C++ , Perl, Python, Lisp, UNIX shell scripting.

Computer Applications: T<sub>E</sub>X (L<sup>A</sup>T<sub>E</sub>X, B<sub>I</sub>B<sub>T</sub>E<sub>X</sub>, P<sub>S</sub>Tricks), most common productivity packages (for Windows, OS X, and Linux platforms), Vim/Vi.

Operating Systems: Microsoft Windows family, Apple OS X, Linux.

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| APPLICATION<br>AREAS | Quantum chemistry theory, Organic based materials, Smart Materials, Biosystem mimic. |
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| CHEMISTRY | Computational and Quantum Theory, Molecular Control, Dynamical processes, Bio-mimics. |
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| MATHEMATICAL | Real and Complex Analysis, Theory of Probability, Linear Algebra, Group Theory. |
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SUMMARY OF  
RESEARCH  
ACTIVITIES

I started my scientific career at the Physical Chemistry Department of the Moscow State University by theoretical studies of carbon based materials (fullerenes and nanotubes). My early research was inspired by the potential use of this class of molecules in organic photovoltaic applications and biological frameworks related to the unique possibility of tuning their electronic properties and solubility via targeted chemical functionalization. In particular, applying broad spectra of theoretical methods (from semiempirical approaches to the density functional theory), I could elaborate a genetic algorithm for prediction of thermodynamically stable or kinetically accessible structures in various classes of poly-functionalized fullerenes systems such as chlorides or perfluoroalkylated derivatives. The strong predictive efficiency of this approach was demonstrated in a number of collaborative works with our synthetic chemistry colleagues, which have been published in several high-impact chemical journals (**Chem. Comm.**, **23**, **2463-5(2006)** , **European J. Org. Chem.** , **5082-94(2007)** , **New J. Chem.**, **32**, **89-93 (2008)**, etc.). In a similar fashion, I have recently provided in a theoretical analysis of very unusual fluorocarbene derivatives of fullerenes ( **Dalton Trans.**,**5322-8(2007)**,**Dalton Trans.**, **48**, **886-93(2008)**). Finally, kinetic characteristics and dynamical nature of structural transformation of fullerene derivatives was understood and analyzed theoretically in **J. Phys. Chem. A**, **113**, **10833-8 (2009)**. Thus, at this stage of my career, I have gained an experience in working together with experimental chemists in solving the problems of the targeted synthesis and structure elucidation of polyfunctionalized fullerenes. My strong contribution to these works was reflected in the first and/or corresponding authorship.

Later this contribution to fullerene chemistry was expanded by a direct translation into continued systems of carbon based materials single walled carbon nanotubes (SWCNT). I have showed that similar schemes as for fullerenes can be applied to SWCNT as well, which is an essential issue in understanding and controlling the electronic structure of SWCNT in a wet-chemistry fashion. It also opens roads to control mechanical properties of SWCNT based Nano Electro Mechanical Systems (NEMS). Under my supervision, results of this work were recently published in high-impact journal in the field of nanomaterials - **ACS Nano**, **4**, **6260-6 (2010)**.

Although computational chemistry is my main field of expertise, I'm also native in many experimental techniques, which is a key point for successful interaction with experimental teams. This is important to make not only fundamental study like one was showed early **Int. J. Mass-Spect.**, **243**, **223-230 (2005)**, but also to propose new ways of materials analysis and fabrication as Ive reported in Novel possibilities in the study of isolated carbon nanotubes published in **Int. J. Mass-Spect.,(rapid)**, **22**, **1372 1376 (2008)**.

After successful PhD defense in 2009, I have won a competition for Erasmus scholarship and started working at the Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology. Here my works are strongly focused on the development of efficient hybrid theoretical methodologies to treat electronic and transport properties of complex materials where dynamical conformational disorder and dynamical nature of matter play a crucial role. My research includes a broad class of materials such as organic molecules, DNA-based oligomers, polymeric systems, and carbon based materials. Among my most recent achievements, I would like to highlight the following:

1) I've proposed theoretical ground for explanation of new phenomenon in organic Zener diode effect where a tunneling across the gap takes place. This work stimulated by experimental observation (in collaboration with Prof. Karl Leo, IAPP), where a strongly asymmetric electric field dependence of the current voltage characteristics of an organic diode has been found. The results of this work have been recently published in **Nano Lett.**, **10**, **4929-4934 (2010)**.

2) I have been strongly involved in the deriving a method for the determination of effective electronic structure parameters in DNA oligomers with different base sequences. This parameterization can be used as a starting point to formulate coarse-grained models for biomolecular systems. The method basically relies on a combined QM/MM mapping of the system of interest. In this work, which has appeared in **Phys. Rev. B**, **82**, **15 (2010)** in particular problems of the DNA mismatching detection was addressed.

3) In collaboration with local colleagues a novel promising ab initio methodology has been developed that will make possible to predict transport properties of organic materials with high accuracy. We obtained strongly positive comments on this approach from several leading workers in this field. It was reported on several valuable conferences like PSI-K Conference(2010), American Chemical Society Meeting(2011) and now has been invited for publication in a special issue of **Israel Journal of Chemistry(accepted, 2011)** devoted to theoretical chemist Stuart A. Rice.

4) In collaboration Molecular Nanostructures group (IFW, Dresden) Dr. Mark H. Rumeli, we carried out the theoretical-experimental research on the in-situ study of molecular systems dynamics where a combination of high resolution transition electron microscopy and molecular dynamics theory are applied for understanding of molecular interaction at the atomic scale (**Nano Res. , 3**, **9297(2010)**).

Also, I have strong collaboration with Electronic Structure of Molecular Materials group (led by Dr. Alexey A. Popov in IFW Dresden). We work together on theoretical studies of endohedral metallofullerenes (**J. Phys. Chem. Letters**, **13**, **1592-00, (2011)**; **J. Phys. Chem. C**, **115**, **3**, **15257-65 (2011)**). These materials are very promising for spitrionic and some bio-medical applications. Recently, theoretically we have proved existence of organometallic complexes of graphene(**ACS Nano**, **2011**, **5 (12)**, **pp 99399949**), which creates more feasible future of graphene based spitronics (spin valve materials, or one atom thin magnets, etc.), and opens new field graphene based webs (submitted, preprint by request). I do believe that in this direction we can continue with long-term collaborative research.

In this respect my knowledge in Materials Modeling along with Biophysical experience make me think that I can have a productively work in Computational Materials Science group broadly defined.

SHORTLY ABOUT  
PLANS

Within the next few years of my research activity, I would like to keep my focus on the plans study of the structural and dynamical properties of complex systems like bio-/organic- based materials. I will try to understand deeper how to control / manipulate upon this molecular chaos and on its energetics and charge dynamics. This topic fascinated me from the beginning for several reasons: Firstly, due to the broad range of computational methodologies to be applied, ranging from classical molecular dynamics simulation techniques to quantum chemical methodologies; secondly, due to the enormous potential that these systems are expected to have in future devices; thirdly because of the lack of a unifying theoretical approach to describe charge migration in them. This later issue represents in my view one of the strongest challenges that scientists working in this field will face in the coming times with regards to sensoric, manipulation and control of these complex systems (biosensors, organic based smart materials). I hope to be able to contribute to these developments. Also, I would love to join to ambipolar team within strongly motivated Department, where both direction of the experimental and theoretical research are growing synchronously. I try to find this productive collaborations, as well as I do believe, that Ill be able to contribute in this framework.

PUBLICATIONS  
SUBMITTED 2012

- 37) Popov A.A., **Avdoshenko S.M.**, Pendas A.M., Dunsch L.  
*Title:* Bonding between strongly repulsive metal atoms: **an oxymoron made real**  
in a confined space of endohedral metallofullerenes  
*link:* by request (2012)
- 36) Boerrnert F., **Avdoshenko S.M.**, Bachmatiuk A., Ibrahim I., Buechner B., Cuniberti G., and Ruemmeli M.H.  
*Title:* Amorphous carbon under 80 kV electron irradiation: A means to make or break graphene  
*link:* by request (2012)
- 35) Nozaki D., Sevincli H., **Avdoshenko S.M.**, Gutierrez R., Cuniberti G.  
*Title:* Control of quantum interference in molecular junctions: Understanding the origin of Fano and anti- resonances with parabolic diagrams  
*link:* <http://arxiv.org/abs/1203.5269> (2012)
- 34) Barreiro A., Boerrnert F., **Avdoshenko S.M.**, Rellinghaus B., Cuniberti G., Ruemmeli M.K., Vandersypen L.M.K.  
*Title:* Transforming amorphous carbon into graphene by current-induced annealing  
*link:* <http://arxiv.org/abs/1201.3131> (2012)

PUBLICATIONS  
2012

- 33) **Avdoshenko S.M.**, Ioffe I.N., Cuniberti G., Dunsch L., Popov A.A.  
*Title:* Correction to Organometallic Complexes of Graphene: Towards Atomic Spintronics Using Graphene Web.  
*link:* *ACS Nano*, 6 (3), 28602860 (2012)
- 32) Kuvychko I., Whitaker J., Larson B., Folsom T., Shustova N., **Avdoshenko S.**, Chen, Yu-S., Wen H., Wang Xue-B., Dunsch L. Popov A., Strauss S., Boltalina O.  
*Title:* Selective Synthesis and Characterization of Ten and their Electron Accepting Properties in Gas Phase and Solution Studied by Low-Temperature Photoelectron Spectroscopy, Cyclic Voltammetry, and DFT Theory.  
*link:* *Chem. Sci., Advance Article*, 2012, *Cover Story*
- 31) **Avdoshenko S. M.**, C.G. Rocha, Cuniberti G.  
*Title:* Nanoscale ears: Graphene Based Nanoscale Sensors  
*Link:* *Nanoscale*, 2012, DOI: 10.1039/C2NR30097D

- 30) Gollub C., **Avdoshenko S. M.**, Gutierrez R., Berlin Y., Cuniberti G.  
*Title:* Charge migration in organic materials: Can propagating charges affect the physical quantities controlling their motion.  
*link:* *Israel Journal of Chemistry*, (2012)
- PUBLICATIONS 2011
- 29) **Avdoshenko S.M.** Ioffe I.N., Cuniberti G., Dunsch L., Popov A.A.  
*Title:* Organometallic Complexes of Graphene: Towards Atomic Spintronics Using Graphene Web.  
*link:* *ACS Nano*, 5 (12), 9939-9949 (2011)
- 28) **Avdoshenko S.M.**  
*Title:* A Multibox Splitting Scheme: Robust Approximation for Ab Initio Molecular Dynamics.  
*link:* *J. Chem. Theory Comput.*, 7 (12), pp 38723883 (2011)
- 27) Kuvychko I., Shustova N., **Avdoshenko S.M.**, Popov A., Strauss S., Boltalina O.  
*Title:* In Search of Fullerene-Based Superacids: Synthesis, X-ray structure and DFT study of  $C_{60}(C_2F_5)_5H$ .  
*Abstract:* **Simply super!** The perfluoroalkylfullerene  $C_{60}(C_2F_5)_5H$  is the first structurally characterized perfluoroalkylated fullerene-based acid and is also predicted to be the first gas-phase fullerene-based **superacid**.  
*link:* *Chemistry - A European Journal*, 17, 8799-8802 (2011)
- 26) Popov A.A., Schiemenz S., **Avdoshenko S.M.**, Yang S., Cuniberti G., Dunsch L.  
*Title:* The State of Asymmetric Nitride Clusters in Endohedral Fullerenes as Studied by  $^{14}N$ -NMR Spectroscopy: Experiment and Theory.  
*link:* *Journal of Physical Chemistry C* 2, 1592 (2011)
- 25) Popov A.A., **Avdoshenko S.M.**, Cuniberti G., Dunsch L.  
*Title:* Dimerization of Radical-Anions: Nitride Clusterfullerenes *vs.* Empty Fullerenes.  
*link:* *Journal of Physical Chemistry Letters*, 2 (13), 1592-1600 (2011 )
- PUBLICATIONS 2010
- 24) **Avdoshenko S.M.**, Ioffe I., Sidorov L.  
*Title:* Smooth and jump-like metal-dielectric transitions in SWCNTs under functionalization.  
*link:* *ACS NANO*, 4, 6260 (2010)
- 23) Lee M. H., **Avdoshenko S.M.**, Gutierrez R., Cuniberti G.  
*Title:* Charge migration through DNA molecules in presence of mismatches.  
*link:* *Physical Review B* 82, 155455 (2010)
- 22) Kleemann H., Gutierrez R., Lindner F., **Avdoshenko S. M.**, Manrique P.-D., Lssem B., Cuniberti G., Leo K.  
*Title:* Organic Zener Diodes: Tunneling across the Gap in Organic Semiconductors.  
*link:* *Nano Letters*, 10, 4929 (2010)
- 21) Gorantla S., **Avdoshenko S.**, Bernert F., Bachmatiuk A., Dimitrakopoulou M., Schaeffle F., Scheonfelder R., Thomas J., Gemming T., Warner J., Cuniberti G., Eckert J., Bchner B., Rummeli M. **2010:** Enhanced  $\pi$  -  $\pi$  interactions between a  $C_{60}$  fullerene and a buckle bend on a double-walled carbon nanotube, *Nano Research*, 3(2), 92-97.
- ISI HIRSCH  
( $H \geq 10$ )
- PUBLICATIONS 2005-2009
- 20) **Avdoshenko S.**, Ioffe I., Sidorov L. **2009:** Theoretical Study of Isomerization Mechanisms in Fluorinated Fullerene Derivatives *J. Phys. Chem. A*, 113(40), 10833-10838

- 19) Goryunkov A., Kornilenko E., Magdeseive A., Kozlov A., Vorobiev V., **Avdoshenko S.**, Ioffe I., Nikitin I., Markov Yu., Khavrel P., Vorobiev A. Sidorov L. **2008**: Electrochemical, ESR and theoretical studies of (6,6)-opened  $C_{60}(CF_2)$ , cis-2- $C_{60}(CF_2)_2$  and their anions, *Dalton Trans.*, 886 - 6893
- 18) **Avdoshenko, S. M.**, Ioffe, I. N., Kozlov, A. A., Markov, V. Y., Nikolaev, E. N., Sidorov, L.N. **2008**: Novel possibilities in the study of isolated carbon nanotubes. *Int. J. Mass. Spectr.*, 22, 1372-1376.
- 17) Khatymov, R. V., Markov, V. Y., Tuktarov, R. F., Ioffe, I. N., Muftakhov, M. V., **Avdoshenko, S. M.**, Pogulay, A. V., Sidorov, L.N. (2008): Electron interaction with  $S_6-C_{60}(CF_3)_{12}$ : Energy pool of fullerene cage. *Int. J. Mass. Spectr.*, 272, 119-126.
- 16) Goryunkov, A., Ioffe, I., Khavrel, P., **Avdoshenko, S.**, Markov, V., MAZEJ, Z., Sidorov, L., Troyanov, S. **2007**: The former  $C_{60}F_{16}$  is actually a double-caged adduct:  $(C_{60}F_{16})(C_{60})$ . *Chem. Commun.*, 704-706.
- 15) Pimenova, A. S., Kozlov, A. A., Goryunkov, A. A., Markov, V. Y., Khavrel, P. A., **Avdoshenko, S. M.**, Ioffe, I. N., Sakharov, S. G., Troyanov, S. I., Sidorov, L.N. **2007**: Synthesis and characterization of difluoromethylene-homo(60)fullerene,  $C_{60}(CF_2)$ . *Chem. Commun.*, , 374-376.
- 14) Goryunkov, A. A., Dorozhkin, E. I., Tamm, N. B., Ignateva, D. V., **Avdoshenko, S. M.**, Sidorov, L. N., Troyanov, S.I. **2007**: Synthesis and molecular structure of 1,6,11,16,18,24,27,36- $C_{60}(CF_3)_8$ . *Mendeleev Commun.*, 110-112.
- 13) Troyanov, S. I., Goryunkov, A. A., Dorozhkin, E. I., Ignateva, D. V., Tamm, N. B., **Avdoshenko, S. M.**, Ioffe, I. N., Markov, V. Y., Sidorov, L. N., Scheurgel, K., Kemnitz, E. **2007**: Higher trifluoromethylated derivatives of  $C_{60}$ ,  $C_{60}(CF_3)_{16}$  and  $C_{60}(CF_3)_{18}$ . Synthesis, structure, and theoretical study. *J. Fluorine Chem.*, 128, 545-551.
- 12) Dorozhkin, E. I., Goryunkov, A. A., Ioffe, I. N., **Avdoshenko, S. M.**, Markov, V. Y., Tamm, N. B., Ignateva, D. V., Sidorov, L. N., Troyanov, S.I. **2007**: Synthesis, structure, and theoretical study of lower trifluoromethyl derivatives of (60)fullerene. **Eur. J. Org. Chem.**, 5082-5094.
- 11) Omelyanyuk, N. A., Goryunkov, A. A., Tamm, N. B., **Avdoshenko, S. M.**, Ioffe, I. N., Sidorov, L. N., Kemnitz E., Troyanov, S.I. **2007**: New trifluoromethylated derivatives of (60)fullerene,  $C_{60}(CF_3)_n$  with  $n = 12$  and  $14$ . *Chem. Commun.*, 4794 - 4796
- 10) Ovchinnikova, N. S., Ignateva, D. V., Tamm, N. B., **Avdoshenko, S. M.**, Goryunkov, A. A., Ioffe, I. N., Markov, V. Y., Troyanov, S. I., Sidorov, L. N., Yurovskaya, M. A., Kemnitz, E. **2007**: Regioselective synthesis and crystal structure of  $C_{70}(CF_3)_{10}[C(CO_2Et)_2]$ . *New J. Chem.*, 32, 89-93
- 9) Pimenova, A. S., Kozlov, A. A., Goryunkov, A. A., Markov, V. Y., Khavrel, P. A., **Avdoshenko, S. M.**, Vorobiev, V. A., Ioffe, I. N., Sakharov, S. G., Troyanov, S. I., Sidorov, L.N. **2007**: Preparation and structures of (6,6)-open difluoromethylene[60]fullerenes:  $C_{60}(CF_2)$  and  $C_{60}(CF_2)_2$ . *Dalton Trans.*, 5322 - 5328.
- 8) Tamm, N. B., **Avdoshenko, S. M.**, Kemnitz, E., Troyanov, S. I. **2007**: Synthesis, Structural Investigation, and Theoretical Study of Pentafluoroethyl Derivatives of (60)Fullerene. *Russ. Chem. Bull.* 56(5), 915-921.
- 7) Markov, V. Y., Aleshina, V. E., Borschevsky, A. Y., Khatyav, R. V., Tuktarov, R. F., Pogulay, A. V., Maximov, A. L., Kardashev, S. V., Ioffe, I. N., **Avdoshenko, S. M.**,

Dorozhkin, E. I., Goryunkov, A. A., Ignat'eva, D. V., Grusinskaya, N. I., Sidorov, L.N. **2006**: Mass spectrometric studies of trifluoromethylated fullerenes. *Int. J. Mass Spect.*, 251, 16-22.

- 6) Ignateva, D. V., Goryunkov, A. A., Tamm, N. B., Ioffe, I. N., **Avdoshenko, S. M.**, Sidorov, L. N., Dimitrov, A., Kemnitz, E., Troyanov, S.I. **2006**: Preparation, crystallographic characterization and theoretical study of the two isomers of  $C_{70}(CF_3)_{12}$ . *Chem. Commun.*, 1778-1780.
- 5) Dorozhkin, E. I., Ignateva, D. V., Tamm, N. B., Vasilyuk, N. V., Goryunkov, A. A., **Avdoshenko, S. M.**, Ioffe, I. N., Sidorov, L. N., Pattison, P., Kemnitz, E., Troyanov, S. I. **2006**: Structure of 1,4,10,19,25,41- $C_{70}(CF_3)_6$ , isomer with unique arrangement of addends. *J. Fluorine Chem.*, 127, 1344-1348.
- 4) Goryunkov, A. A., Ignateva, D. V., Tamm, N. B., Moiseeva, N. N., Ioffe, I. N., **Avdoshenko, S. M.**, Markov, V. Y., Sidorov, L. N., Kemnitz, E., Troyanov, S.I. **2006**: Preparation, Crystallographic Characterization and Theoretical Study of  $C_{70}(CF_3)_{14}$ . *Eur. J. Org. Chem.*, 2508-2512.
- 3) **Avdoshenko, S. M.**, Goryunkov, A. A., Ioffe, I. N., Ignat'eva, D. V., Sidorov, L. N., Pattison, P., Kemnitz, E., Troyanov, S.I. **2006**: Preparation, crystallographic characterization and theoretical study of  $C_{70}(CF_3)_{16}$  and  $C_{70}(CF_3)_{18}$ . *Chem. Commun.*, 2463-2465.
- 2) Goryunkov, A. A., Kareev, I. E., Ioffe, I. N., Popov, A. A., Kuvychko, I. V., Markov, V. Y., Gold, I. V., Pimenova, A. S., Serov, M. G., **Avdoshenko, S. M.**, Khavrel, P. A., Sidorov, L. N., Lebedkin, S. F., Mazej, Z., Zemva, B., Strauss, S. H., Boltalina **2006**: Reaction of  $C_{60}$  with  $KMnF_4$ . Isolation and characterization of a new isomer of  $C_{60}F_8$  and re-evaluation of the structures of  $C_{60}F_7(CF_3)$  and the known isomer of  $C_{60}F_8$ . *J. Fluorine Chem.*, 127, 1423-1435.
- 1) Ioffe, I., **Avdoshenko, S.**, Boltalina, O., Sidorov, L., Berndt, K., Weber, J., Kappes, M. **2005**: Photoelectron Spectroscopy and Quantum Chemical Studies of  $C_{60}F_{34}^{2-}$ . *Int. J. Mass. Spect.*, 243, 223-237.

#### CONFERENCE TALKS

- S. M. Avdoshenko, et al. *DNA Translocation through Nanopores and the Sequencing Problem: A Theoretical Study*, **EUROMAT, 2011**, Montpellier, France.
- S. M. Avdoshenko, *Time-space resolved charge dynamics in complex systems*, **Novel Simulation Approaches to Soft Matter Systems, 2010**, Dresden.
- S. M. Avdoshenko, *Real time/space charge dynamics in complex systems*, **PSI-K Conference, 2010**, Berlin.
- S. M. Avdoshenko, *Computational Approach for the Searching of Promising Fullerenes and Nanotubes Derivatives*, **ANSYS Conference and CADFEM Users Meeting, 2007**, Dresden.

#### REFERENCES

- Prof. G. Cuniberti (collaboration since March 2009), TU Dresden, Germany  
[g.cuniberti@nano.tu-dresden.de](mailto:g.cuniberti@nano.tu-dresden.de)  
 Dr. I. Ioffe (PhD direct supervisor), MSU, Russia  
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 Dr. A. Popov (collaboration), IFW. Dresden  
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