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EDUCATION:

1998 **Ph.D. (physical and mathematical sciences), Moscow State University, Moscow, Russia**

- Ph.D. thesis "Direct and resonant charge-exchange processes of fast ions and their slowing-down kinetics at propagation through matter", sc. advisor prof. V.V.Balashov
- fellowship from the International Soros Science Education Program (ISSEP) for PhD students (1996)

1995 **Master of Science (physics), Moscow State University, Faculty of Physics, Moscow, Russia**

- M.Sc thesis "Electronic structure of channeled hydrogen-like ions at energies of tens and thousands MeV"
- Graduated with honors

1989 **Specialized secondary school for physics and mathematics at Kiev State University, Kiev, USSR**

WORK EXPERIENCE:

2019-present time **Researcher at the Italian National Research Council (CNR-IOM), Italy**

- I work within the project “Diffusive transport and absorption in nanoporous materials” aimed at establishing predictive diffusive models for nano-porous systems in cell biology (transport though cell membranes) and material science (gas transport and absorption in nano-porous materials).
- My duties include: all-atom molecular dynamic simulations (including force field generation, system design, and data analysis) the transport of molecule through the nano-scale pores using both standard and enhanced sampling methods (metadynamics); development of the diffusion-scale models of transport and bridge the parameters with the all-atom simulations; analyze the experimental data and bridge the results with the simulations.
- **Teaching activity**
  December, 2019 – course of general physics for nursing students, University of Cagliari, Cagliari, Italy.

2014-2019 **Researcher at the Department of Physics, University of Cagliari, Italy**

- I participated in the “Translocation” consortium (http://www.nd4bb.eu) aimed at establishing the molecular basis of antibiotic translocation through cell membranes that received support from the Innovative Medicines Initiative, a joint undertaking between the European Union and the pharmaceutical industry association, EFPIA. Group leader – Prof. Matteo Ceccarelli.
- My duties included modeling of molecular (antibiotic) transport through porins in outer membranes of Gram-negative bacteria at various scales - from the MD scale to the diffusion models. In particular, the aim was to design an adequate Markov state model and a diffusion-drift model of the translocation process (used to compare with the experimental data) and the protocols to calculate the parameters of the model from the atomistic simulations. The work assumed both development of the methods and the software as well as and the applied simulations.
- We developed an improved statistical method to analyze the kinetics of the molecule-porin iteration in the single-channel electrophysiology experiments, which extends the sensibility of the experimental method to the nanosecond time scale. We developed a novel computational method to quantify the macroscopic electric field around solvated macromolecules directly from all-atom MD simulations. We suggested a new mechanism of passing transport and developed a quantitative model of filtering of polar molecules by porins taking into account the

steric barrier in the constriction region of the channel and its strong internal electric field. Based on the model, we designed a scoring function for fast prediction of permeability of general porins of *Enterobacteriaceae* family to polar molecules.

- **Teaching activity**
  July, 2015 – tutorial "Statistical grounds of the analysis of the substrate-pore interaction in the single-channel electrophysiology experiment" (4 hours) at the ITN "Translocation" summer school, Jacobs University Bremen, Bremen, Germany;
  November, 2017 – special course "Physical grounds of the interaction of ionizing radiation with living matter" (4 hours) for the students of Medical Imaging, Radiology and Radiotherapy, University of Cagliari, Cagliari, Italy.
  November, 2018 – course of general physics for nursing students, University of Cagliari, Cagliari, Italy.
  Scientific co-advisor of PhD students: Tommaso D'Agostino (2016), S Salis (2017), S. Acosta-Gutierrez (2017)

2010-2013 Researcher at the National Nanotechnology Laboratory (NNL, CNR-NANO), Lecce, Italy

- I participated in the DEDOM (**De**velopment of **D**ensity Functional Methods for **O**rganic-**M**etal Interaction) project funded by the European Research Council as a Starting Grant for independent research. DEDOM is a theoretical research project that aimed to develop new Density Functional Theory (DFT) methods to describe the interaction between organic molecules and noble metal substrates, team leader – Dr. Fabio Della Sala.
- My duties included development of the hybrid quantum-mechanical/molecular mechanical (QM/MM) methods for molecule-metal surface interactions and their implementation within TURBOMOLE ab-inito software packages.
- We have developed an extension of the charge-dipole model for the description of periodic systems. This periodic charge-dipole electrostatic model (PCDEM) allows one to describe the linear response of periodic structures in terms of charge- and dipole-type Gaussian basis functions. The long-range electrostatic interaction is efficiently described by means of the continuous fast multipole method. As a first application, the PCDEM method was applied to describe the polarizability of silver slabs. We found that for a correct description of the polarizability of the slabs both charges and dipoles are required. However, a continuum set of parametrizations, i.e., different values of the width of charge and dipole-type Gaussians, leads to an equivalent and accurate description of the slabs polarizability but a completely unphysical description of induced charge-density inside the slab. We introduced the integral squared density measure that allows one to obtain a unique parametrization which accurately describes both the polarizability and the induced density profile inside the slab. Besides, we have developed a simple method to include the kinetic-exchange-correlation (KXC) correction to the charge-dipole polarizable electrostatic model. On the example of 2D-periodic silver slabs, we show that the KXC-correction to the periodic charge-dipole electrostatic model significantly improves the description of the linear response of the slabs to an external electrostatic perturbation. The profiles of the plane-integrated induced 1D-charge density as well as the response electric field of the slabs can be described with the accuracy close the limit accuracy of the charge-dipole Gaussian basis set.
- The PCDEM-KXC model has been formally extended to time-dependent perturbations for finite clusters and implemented within TURBOMOLE program.

2008 – 2010 Senior Research Fellow at the Institute of Nuclear Physics, Moscow State University, Moscow, Russia

- I participated (group leader - Dr. Eugene Tkalya) in the project on multiscale simulation of molecular systems and nanostructured materials. The project follows the idea of consistent treatment at different time and spatial scales – from high-level ab-initio quantum mechanical calculations for 50-100 atoms to the force field or semiempirical methods for up to 10000 atoms and further to the thermodynamic simulation of the macroscopic properties.
- My duties included
  - general coordination of the project
  - theoretical development and computer implementation of the advanced methods of ab-initio and semiempirial quantum chemistry
  - maintenance and development of our original computer program for quantum chemical calculations
- The problems within the project included
  - Multiscale simulation of the adsorption of molecular hydrogen in carbon-based nanostructures, modification and optimization of the adsorbent materials for potential

use as a hydrogen storage medium. The hydrogen-material interaction energy from the ab-initio quantum chemistry (HF, MP2, and basis set convergence) was used fit the force field; the force field was used then in the thermodynamic simulation to calculate the hydrogen adsorption capacity of the material.

- Based on first-principles calculations of molecular electron structure, we have suggested the strategy of modifying the carbon-based materials in order to increase their capacity to bind with molecular hydrogen.
- Ab-initio calculations of the electronic excitations in molecules and nanostructures. We have performed pioneer non-empirical (Hartree-Fock) multiconfiguration calculation of the optical electronic excitations in the fullerene C_{60} molecule
- Study of the influence of the electronic (chemical) state of the material on the nuclear reactions. In particular, we investigated the electron capture β decay of ^{7}Be located inside and outside the C_{36} fullerene and found that the ^{7}Be half-life in the $^{7}Be@C^{36}$ molecular complex is expected to be the largest among those known up to date. In addition, we suggested a new mechanism of electron density enhancement (and increase on the β decay rate) on the Be nucleus located in the C60 fullerene. We studied the probability of electron capture by the ^{7}Be nucleus in the ^{7}BeO crystal and the β phase of the $^{7}Be(OH)_2$ crystal modeled as clusters subjected to external pressure. Calculated rates of the increase of the ^{7}Be nuclear decay constant λ with pressure in these compounds are substantially smaller than the values found experimentally, in agreement with the DFT calculations by other groups. We discussed possible reasons for discrepancy between the theory and the experiment.

2002-2008 Senior Research Fellow at Algodign™, LLC – U.S. start-up company established to develop novel software for structure-based drug design, based on advanced methods of physics with the research operations primarily conducted in Russia

- I initiated, argued in favor of and lead the ab-initio quantum chemistry project. In brief, the reasoning follows. The force field for the biomolecular simulations must take account of both hard and soft intra- and intermolecular interactions including the hydrogen bonding, the dispersion and the aromatic interactions, charge transfer through the molecule, etc. To design and fit it from the first principles one needs the results of the quantum mechanical calculations of the interaction energy of molecular fragments containing up to 50-100 atoms at numerous configurations with the overall accuracy better than 0.5 kcal/mol. Then, the quantum theory level must be at least Hartree-Fock + MP2, while the basis set convergence must be studied as well. Therefore, the quantum chemical software must be capable to perform 1 PC calculations of up to 50-100 atoms with up to 2000-4000 basis functions within few days. That was not possible with existing commercial software (e.g., GAMESS, GAUSSIAN, JAGUAR), therefore the quantum chemistry project was initiated at Algodign.
- By implementing the recently developed methods (e.g., the resolution of the identity), our original algorithms and efficient basis sets, we had achieved the goal. Our program (called AlgoQMT) designed completely in my group of 3-5 physicists may be by more than 10 time faster than GAMESS and by more than 2-3 times than JAGUAR at the same accuracy level. The program includes the following modules
  - The library routines for calculating various molecular integrals
  - The Hartree-Fock solver and electronic properties
  - MP2 and electronic properties
  - Configuration interaction (CI) and electronic properties
  - Molecular geometry optimization, harmonic modes analysis and anharmonic corrections
  - Efficient series of the RI basis set for convergent calculations
  - Electronic density maps for selected orbitals for visualizing the nature of molecular interactions
- Another group used the AlgoQMT program for the parameterization of the polarizable force field QMPFF designed at Algodign.
- I also took part in calculations and/or discussions on most projects carried out at Algodign. Thereby, I have got the understanding of the most stages and methods of the structure based drug design – both empirical, e.g., virtual screening, docking, scoring functions (knowledge based and binding/activity constants based), in situ ligand design by linking or by fragment growing, etc. – and physics based, e.g. force field design and fitting, molecular dynamics simulation of protein-ligand binding free energy, etc.
- We had lectures, tutorials and numerous discussions with the world-class experts in proteins and bio simulations – Prof. Michael Levitt and Prof. Alexei Finkelstein. We had also lectures on

drug design and simulations by Dr. Jay Ponder and Dr. Philip Payne.

1998-2002 **Postdoctoral research associate at the Institute of Nuclear Physics, Moscow State University, Moscow, Russia**

- I developed the theory, designed the computer program and performed calculations of the (e,2eγ) and (e,3e) experiments as 'perfect experiments' to study the ionization-excitation process in electron-atom collisions. Advancements in coincidence measurements in atomic collisions had made it possible a 'perfect experiment'. That is, one can obtain the maximum available information on a quantum system – determine its wavefunction and transition amplitudes. We addressed the ionization-excitation process of atoms by electron, photon and heavy-particle impact -- the topical issue in the atomic collisions physics of that time, – when a fast particle ionize the target atom leaving the residual ion in the excited (possibly autoionizing) state. In particular, we performed a detailed first principles theoretical analysis of the electron impact ionization-excitation of helium and argon atoms and determined for the first time the conditions of the 'perfect experiment' providing suggestions and guides for upcoming experiments.
- I developed a statistical theory of the slowing down and angular dispersion of a beam of fast ions in matter taking into account the dynamics of ionic states. The theory and computer programs were developed for detailed studies of the energy-loss and angular distributions and the energy deposition profiles of heavy fast ions passing through matter taking into account the electron capture and loss processes. In particular, a quantitative explanation of the non-trivial two-bump form of the energy loss distributions of fast lithium ions passing through very thin carbon films was given for the first time.
- I developed the theory, designed the computer program and performed calculations for the density-matrix approach to theoretical investigation of the resonant coherent excitation (RCE) of channeled ions (the Okorokov effect).
- I designed the computer program and performed calculations for the problem of evolution of the spin density matrix of a quantum system (atoms, atomic ions) in the course of an arbitrary branching cascade of electromagnetic transitions.
- Professional awards and fellowships
  - 2001 – awarded by the Stipend of the Scientific Council of Moscow State University for Young Scientists Having Achieved Essential Results in Scientific Research and Teaching
  - 2000 – noted by a valuable gift of the rector of Moscow State University;
  - 1999 – the 1st award at the Contest of Scientific Papers by Young Scientists of the Institute of Nuclear Physics, Moscow State University
- Teaching activity
  - 1998 – a special course 'The practice on numerical methods' for the students of the Physics of Atomic Nucleus Chair at the Physics Faculty of Moscow State University;
  - 1999 – a special course 'Kinetic equations of the theory of interaction of radiation with matter' for the students of the Physics of Atomic Nucleus Chair at the Physics Faculty of Moscow State University.
- Grants participation
  - 1998-99 – a principal investigator of the project 'Direct and resonant charge-exchange processes and slowing down kinetics of fast ions passing through thin slices of matter' supported by the Federal Program 'Universities of Russia – Basic Research'; grant #5364.
  - 2000-02 – participated projects # 00-02-17207 and № 01-02-06248 supported by the Russian Foundation for Basic Research (RFBR), the second one – as a principal investigator.

VISITING POSITIONS:

October – December 2009 **Service de physique non-lineair et mechanique statisique, Universite Libre de Bruxelles (Brussels, Belgium) – visiting researcher, group of Prof. D.Kosov**

- quantum transport in nanoscale molecular systems

July – October 2009 **Physics Institute, Heidelberg University (Heidelberg, Germany) – visiting researcher, group of Dr. A.Surzhykov**

- formation of quasi-molecules in slow heavy-ion collisions

List of journal publications and book chapters

1. Jayesh Arun Bafna, Eulalia Sans-Serramitjana, Silvia Acosta-Gutierrez, Igor V Bodrenko, Daniel Hörömpöli, Anne Berscheid, Heike Broetz-Oesterhelt, Mathias Winterhalter, Matteo Ceccarelli, “Kanamycin Uptake into *Escherichia coli* Is Facilitated by OmpF and OmpC Porin Channels Located in the Outer Membrane”// ACS Infectious Diseases, xxxx (2020); DOI:10.1021/acsinfecdis.0c00102
2. Domenica Farci, Mehmet Alphan Aksoyoglu, Stefano Francesco Farci, Jayesh Arun Bafna, Igor Bodrenko, Matteo Ceccarelli, Joanna Kirkpatrick, Mathias Winterhalter, Sami Kereïche, Dario Piano, “Structural insights into the main S-layer unit of Deinococcus radiodurans reveal a massive protein complex with porin-like features”//Journal of Biological Chemistry, 295 (2020) 4224-4236; DOI: 10.1074/jbc.RA119.012174
3. *Julia Vergalli, Igor V Bodrenko, Muriel Masi, Lucile Moynié, Silvia Acosta-Gutiérrez, James H Naismith, Anne Davin-Regli, Matteo Ceccarelli, Bert van den Berg, Mathias Winterhalter, Jean-Marie Pagès, “Porins and small-molecule translocation across the outer membrane of Gram-negative bacteria”// Nature Reviews Microbiology, 18,164–176 (2020); DOI: 10.1038/s41579-019-0294-2
4. D. Benkerrou, V. Minicozzi, A. Gradogna, S. Milenkovic, I.V. Bodrenko, M. Festa, L. Lagostena, L. Cornara, A. D'Amore, M. Ceccarelli, A. Filippini, A. Carpaneto, “A perspective on the modulation of plant and animal two pore channels (TPCs) by the flavonoid naringenin” //Biophysical Chemistry, 254 (2019) 106246; DOI:10.1016/j.bpc.2019.106246
5. *Igor V Bodrenko, Samuele Salis, Silvia Acosta-Gutierrez, Matteo Ceccarelli, “Diffusion of large particles through small pores: From entropic to enthalpic transport”// J. Chem. Phys., 150 (2019) 211102; DOI: 10.1063/1.5098868
6. Joan Coines, Silvia Acosta-Gutierrez, Igor Bodrenko, Carme Rovira and Matteo Ceccarelli, “Glucose transport via the pseudomonad porin OprB: implications for the design of Trojan-horse antinfectives”// Physical Chemistry Chemical Physics, 21, 8457 (2019); DOI: 10.1039/c9cp00778d
7. *Samanta, Susruta; Bodrenko, Igor; Acosta-Gutierrez, Silvia; D'Agostino, Tommaso; Pathania, Monisha; Ghai, Ishan; Schleberger, Christian; Bumann, Dirk; Wagner, Richard; Winterhalter, Mathias; van den Berg, Bert; Ceccarelli, Matteo, "Getting large drugs through small pores: exploiting the porins pathway in Pseudomonas aeruginosa" // ACS Infectious Diseases, 4,1519 (2018); DOI:10.1021/acsinfecdis.8b00149
8. Acosta-Gutierrez, Silvia; Ferrara, Luana; Pathania, Monisha; Masi, Muriel; Wang, Jiajun; Bodrenko, Igor; Zahn, Michael; Winterhalter, Mathias; Stavenger, Robert; PAGES, Jean-Marie; Naismith, James; van den Berg, Bert ; Page, Malcolm; Ceccarelli, Matteo, “Getting drugs into Gram-negative bacteria: Rational rules for permeation through porins" // ACS Infectious Diseases, 4, 1487 (2018);DOI:10.1021/acsinfecdis.8b00108
9. Carlo Guardiani, Andrea Magrì, Andonis Karachitos, Maria Carmela Di Rosa, Simona Reina, Igor Bodrenko, Angela Messina, Hanna Kmita, Matteo Ceccarelli, Vito De Pinto, “yVDAC2, the second mitochondrial porin isoform of Saccharomyces cerevisiae”// Biochimica et Biophysica Acta (BBA)-Bioenergetic, 1859, 270 (2018)
10. *Igor V. Bodrenko, Jiajun Wang, Samuele Salis, Mathias Winterhalter, and Matteo Ceccarelli, “Sensing Single Molecule Penetration into Nanopores: Pushing the Time Resolution to the Diffusion Limit”//ACS Sensors, 2, 1184 (2017)
11. Harsha Bajaj, Silvia Acosta-Gutierrez, Igor Bodrenko, Giuliano Malloci, Mariano Andrea Scorciapino, Mathias Winterhalter, and Matteo Ceccarelli, “Bacterial Outer Membrane Porins as Electrostatic Nanosieves: Exploring Transport Rules of Small Polar Molecules”//ACS Nano, 11, 5465 (2017)
12. Ishan Ghai, Alessandro Pira, Mariano Andrea Scorciapino, Igor Bodrenko, Lorraine Benier, Matteo Ceccarelli, Mathias Winterhalter, and Richard Wagner, “General Method to Determine the Flux of Charged Molecules through Nanopores Applied to β-Lactamase Inhibitors and OmpF”// J. Phys. Chem.Lett., 8, 1295 (2017)
13. Mariano Andrea Scorciapino, Silvia Acosta-Gutierrez, Dehbia Benkerrou, Tommaso D’Agostino, Giuliano Malloci, Susruta Samanta, Igor Bodrenko, Matteo Ceccarelli, “Rationalizing the permeation of polar antibiotics into Gram-negative bacteria”// J. Phys.: Condens. Matter, 29, 113001 (2017)
14. Mariano Andrea Scorciapino, Tommaso D'Agostino, Silvia Acosta-Gutierrez, Giuliano Malloci, Igor Bodrenko, Matteo Ceccarelli, “Exploiting the porin pathway for polar compound delivery into Gram-negative bacteria” // Future Medicinal Chemistry, 8, 1047, (2016)

15. S.A. Gutiérrez, I. Bodrenko, M.A. Scorciapino, M. Ceccarelli, “Macroscopic electric field inside water-filled biological nanopores” // Physical Chemistry Chemical Physics 18 (13), 8855 (2016)
16. Silvia Acosta-Gutierrez, Mariano Andrea Scorciapino, Igor Bodrenko, and Matteo Ceccarelli, “Filtering with Electric Field: The Case of E. coli Porins” // J. Phys. Chem. Lett., 6, 1807 (2015)
17. A.V. Avdeenkov, I.V. Bodrenko, D.G. Bessarabov, A.V. Bibikov, A.V. Nikolaev, M.D. Taran, A. Tokarev, E.V. Tkalya, “Thermodynamical model for hydrogen storage capacity in carbon nanostructures”// International journal of hydrogen energy 40, 4184 (2015)
18. *Igor Bodrenko, Harsha Bajaj, Paolo Ruggerone, Mathias Winterhalter and Matteo Ceccarelli, “Analysis of fast channel blockage: revealing substrate binding in the microsecond range”// Analyst 140, 4820 (2015)
19. A.V. Bibikov, A.V. Avdeenkov, I.V. Bodrenko, A.V. Nikolaev, and E.V. Tkalya, Reply to “Comment on ‘Theoretical study of the pressure effect on the electron-capture β decay of ^{7}Be in ^{7}BeO and ^{7}Be(OH)$_2$’ // PHYSICAL REVIEW C **90**, 019802 (2014)
20. *I.V. Bodrenko and F. Della Sala, A periodic charge-dipole electrostatic model. II. A kinetic-exchange-correlation correction // THE JOURNAL OF CHEMICAL PHYSICS 139, 144109 (2013)
21. A.V. Bibikov, A.V. Avdeenkov, I.V. Bodrenko, A.V. Nikolaev, and E.V. Tkalya, Theoretical study of the pressure effect on the electron-capture β decay of ^{7}Be in ^{7}BeO and ^{7}Be(OH)$_2$ // PHYSICAL REVIEW C 88, 034608 (2013)
22. E.V. Tkalya, A.V. Avdeenkov, A.V. Bibikov, I.V. Bodrenko, and A.V. Nikolaev. Electron capture beta decay of Be-7 located inside and outside the c-36 fullerene. *Physical Review C - Nuclear Physics*, 86(1):014608(7) (2012)
23. *I.V. Bodrenko, A.V. Avdeenkov, D.G. Bessarabov, A.V. Bibikov, A.V. Nikolaev, M.D. Taran, and E.V. Tkalya, “Hydrogen storage in aromatic carbon ring based molecular materials decorated with alkali or alkali-earth metals“// *Journal of Physical Chemistry C*, 116, 25286 (2012)
24. *I.V. Bodrenko, M. Sierka, E. Fabiano, and F. Della Sala, “Periodic Charge-Dipole Electrostatic Model using the Fast-Multipole Method: Parametrization of Silver Slabs”// J.Chem.Phys. 137, 134702 (2012)
25. Lucian A. Constantin, Letizia Chiodo, Eduardo Fabiano, Igor Bodrenko, and Fabio Della Sala “Correlation energy functional from jellium surface analysis”// PHYSICAL REVIEW B 84, 045126 (2011)
26. A. V. Nikolaev, I. V. Bodrenko, A. V. Bibikov and E. V. Tkalya, “Configuration interaction calculations of molecular electronic excitations and optical transitions in C60” // in “The Carbon Nanoworld: From Graphene to Nanotubes”, 2011: 175-191; ISBN: 978-81-7895-516-2 Editors: Alvaro W. Mombrú and Mauricio Terrones
27. *E. V. Tkalya, A. V. Bibikov and I. V. Bodrenko, “Electron capture β decay of ^{7}Be encapsulated in C_{60}: Origin of increased electron density at the ^{7}Be nucleus”// PHYSICAL REVIEW C 81, 024610-6 (2010)
28. A.V.Avdeenkov, A.V. Bibikov, I.V. Bodrenko, A.V. Nikolaev, E. V. Tkalya, “Modified carbon nanostructures as hydrogen storage materials”// Russian Physics Journal, Vol. 52, No. 11, 2009, pp.1235-1241.
29. A.V. Nikolaev, A.V. Bibikov, I.V. Bodrenko, A.V.Avdeenkov, E. V. Tkalya, “Electronic and transport properties of rectangular graphene macromolecules and zigzag carbon nanotubes of finite length” // PHYSICAL REVIEW B79 (2009), pp. 045418-1 (-6)
30. V.V.Balashov, V.K.Dolinov, I.V.Bodrenko, A.A.Sokolik, A.V.Stysin, “Density matrix description of resonant coherent excitation of swift highly charged ions in oriented crystals” // Journal of Physics: Conference Series 163 (2009) 012087
31. A. V. Nikolaev, I.V.Bodrenko, E. V. Tkalya, “Theoretical study of molecular electronic excitations and optical transitions of C60” // PHYSICAL REVIEW A 77 (2008), pp. 012503-1 (-7)
32. *V.V.Balashov, I.V.Bodrenko, “Characteristic X-ray production in the RCE process” // Physics Letters A 352 (2006) 129–132
33. *V.V.Balashov, I.V.Bodrenko, “Metastable ion production in the RCE process” // Nuclear Instruments and Methods in Physics Research B 245 (2006) 52–55
34. Alexander Artemyev, Anton Bibikov, Igor Bodrenko, Valentin Zayets, ”Basis set convergence studies of Hartree–Fock calculations of molecular properties within the resolution of the identity approximation” // THE JOURNAL OF CHEMICAL PHYSICS, 2005, v. 123, pp. 024103-1 (-11)
35. *V.V.Balashov, L.L.Balashova, I.V.Bodrenko, “Kinetics of stopping of fast protons propagating through oriented crystalline target”// Yadernaya Phizika, 2002, v.65, №3, pp. 435-439 (in Russian); Physics of Atomic Nuclei, 2002, v.65, №3, pp.409-412.
36. *V.V.Balashov, A.V.Bibikov, I.V.Bodrenko, “Mean charge of highly charged ions passing through matter in the non-equilibrium mode” // Bulletin of Moscow University, Series Physics Anstronomy, 2002, N2, pp.28-32 (in Russian)
37. V.V.Balashov, I.V.Bodrenko, A.Lahmam-Bennani, “(e,3e) as a two-step process” // In "Many Particle Spectroscoppy of Atoms, Molecules , Clusters and Surfaces" ed. J. Kirshner and J. Berakdar, Kluwer Academic /Plenum Publishers, 2001, pp. 283-290, ISBN: 978-1-4613-5491-8 (Print) 978-1-4615-1311-7 (Online)
38. *V.V.Balashov, I.V.Bodrenko, “Angular anisotropy of characteristic radiation of channeled ions at resonant coherent excitation” // Bulletin of Moscow University, Series Physics Anstronomy, 2001, N1, pp.27-30 (in Russian)

39. *V.V.Balashov, I.V.Bodrenko, “Triple coincidence (e,2eγ) measurements as a 'perfect experiment' instrument in ionization-excitation studies” // Journal of Physics, ser. B, 1999, v.32, pp.L687-L692. (Corrections – Journal of Physics, ser. B, 2000, v.33, p.1473)
40. *V.V.Balashov, I.V.Bodrenko, ”Charge-exchange effects in angular resolved energy-loss spectra of HCI propagating through matter” // Physica Scripta, v. T80,1999, p.254-255
41. *V.V.Balashov, A.V.Bibikov, I.V.Bodrenko, “Charge-exchange effects in the energy and angular distributions of fast multiply charged ions propagating through matter”// Bulletin of Russian Academy of Sciences, Physical Series, V. 62, 1998, pp. 734-743
42. *V.V.Balashov, A.V.Bibikov, I.V.Bodrenko, “Charge-exchange effects in energy distributions of fast highly charged propagating through matter”// Russian JETP, V.84(6), June 1997, pp.1215-1220
43. *V.V.Balashov, I.V.Bodrenko, “Non-equilibrium energy-loss spectra of fast ions propagating through matter”// Physics Letters A, v.232, 1997, p.231-233
44. V.V.Balashov, I.V.Bodrenko,V.K.Dolinov, S.I.Strakhova, “Angular anisotropy of cascade photons the course of dielectronic recombination of ions”// Optika i Spektroskopiya, 1994, V.77, N6, pp.891-897 (in Russian); Optics and Spectroscopy, 1994, v.77, № 6, pp.801-806

Patent applications.

1. I.V.Bodrenko, E.V.Tkalya, A.V.Bibikov, C.Queen, METHOD FOR STORING HYDROGEN USING NOVEL CARBON-BASED HIGH CAPACITY STORAGE MATERIALS, Patent application, (International application number PCT/US2007/024101)
2. I.V.Bodrenko, E. V. Tkalya, “Detector of ionizing radiation with nanotubes as sensitive elements” // patent №2311664 (Russia), 2006

Preprints.

1. V. I. Kukulin, A. V. Bibikov, E. V. Tkalya, M. Ceccarelli, I. V. Bodrenko**,** “^{7}Be and ^{22}Na radionuclides for a new therapy of cancer” // arXiv:1907.05934 [physics.med-ph]
2. IV Bodrenko, S Salis, S Acosta-Gutierrez, M Ceccarelli, “Diffusion of large particles through small pores: from entropic to enthalpic transport” // arXiv preprint arXiv:1805.12541 (2018)
3. SN Yudin, IV Bodrenko, G Ya Korenman, “Interaction between antiprotonic helium ion and He atom: Potential Energy Surface”//arXiv preprint arXiv:1612.03874 (2016)

Conference presentations.

1. I.V.Bodrenko and M.Ceccarelli, “Molecular Transport Through Nanopores: Bridging Simulations and Experiment”//oral presentation, CECAM workshop: “Challenges in Large Scale Biomolecular Simulations 2019: Bridging Theory and Experiments”, Institut d'Études Scientifiques de Cargèse, (France), 13-17.05.2019
2. I.V.Bodrenko and M.Ceccarelli, “Filtering molecules with electrostatic”//oral presentation, 104o Congresso Nazionale della Societá Italiana di Fisica, Cosenza (Italia), 17-21.09.2018
3. I.V.Bodrenko and M.Ceccarelli, “Molecular transport through flexible nanochannels: the origin of the entropic barrier” // poster presentation, workshop “Nanofluidics in physics and biology”, Lyon (France), 9-12.06.2018
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