Dr. Maria E. Gracheva

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Education:

- Ph.D. in Solid State Physics (Candidate in Physics and Mathematics) (1998), Moscow State Engineering Physics Institute (MEPhI) Technical University, Russia
- M.S. (Engineer-Physicist) in Solid State Physics (1995), MEPhI, Russia

Employment:

- (August 2008 - current) Assistant Professor, Department of Physics, Clarkson University (Potsdam, New York),
- (2004-summer 2008) Postdoctoral Associate with Professor Jean-Pierre Leburton, Beckman Institute for Advanced Science and Technology, University of Illinois (Urbana-Champaign)
- (2001-2003) Postdoctoral Associate with Professor Hans Othmer, Department of Mathematics, University of Minnesota Instructor in Precalculus
- (1999-2001) Postdoctoral Associate with Professor James D. Gunton, Department of Physics, Lehigh University Teaching Assistant, Laboratory instructor
- (1997-1998) Graduate student, Research and Teaching Assistant, Department of Physics and Technical Application of Superconductivity, MEPhI Fellowship of Genius Student Program of Samsung Electronics Corporation

Research Interests:

Bionanotechnology, Biophysics and Solid State Physics with an emphasis on large scale and multi-scale computations

Experience in the following topics: Ion/charged molecule filtering with a semiconductor nanopore; Semiconductor device electrostatics; DNA characterization with nanopore semiconductor device; Artificial ion channels; Cell-cell communication, inter/intracellular signaling networks; Cell motility; Cell-Extracellular Matrix interaction; Gas-liquid and liquid-solid phase transitions; free energy functionals; Superconductivity, high-temperature superconductivity, vortex system in high-temperature superconductors (HTSC), phase transitions and dynamics of vortex system in HTSC with defects.

Computational background
Monte Carlo and Molecular Dynamics on canonical and grand canonical ensembles, constant pressure ensembles; Biasing techniques to sample infrequent events, histogram reweighting technique; Supercomputing/parallel programming experience; Numerical integration of PDEs, ODEs; Stochastic modeling of PDEs; Electrostatic calculations with Poisson equation; Multi-scale techniques.

Publications:

1. "Simulation of ionic current through the nanopore in a double-layered semiconductor membrane", A. Nikolaev, M. Gracheva, *Nanotechnology* **22**(16), p. 165202 (2011).

2. "DNA characterization through semiconductor layered membranes", D.V. Melnikov, J.-P. Leburton, M.E. Gracheva, Book Chapter in "Nanopore-based technology: single molecule characterization and DNA sequencing", edited by M.E. Gracheva, p. - , Humana Press 2011.

3. "Simulation of electronic sensing of biomolecules in translocation through a nanopore in a semiconductor membrane", M.E. Gracheva, A. Leroux, J. Destine, J.-P. Leburton, Book Chapter in "Nanopores: sensing and fundamental biological interactions", edited by S.M. Iqbal and R. Bashir, p. - , Springer 2010.

4. "SPICE-circuit simulation of the electrical response of semiconductor membrane to a single-stranded DNA translocating through a nanopore", A. Leroux, J. Destine, B. Vanderheyden, M.E. Gracheva, J.-P. Leburton, *IEEE Transactions on Nanotechnology* **9**(3), p. 322-329 (2010).

5. "A model of fibroblast motility on substrates with different rigidities", I. Dokukina, M. Gracheva, *Biophysical Journal* **98**(12), p. 2794-2803 (2010).

6. "Multilayered semiconductor membranes for nanopore ionic conductance modulation", M.E. Gracheva, D.V. Melnikov and J.-P. Leburton, *ACS Nano* **2**(11), p. 2349-2355 (2008).

7. "Simulation of electrically tunable semiconductor nanopores for ion current/single bio-molecule manipulation", M.E. Gracheva, J.-P. Leburton, *J. Comput. Electronics* **7**(1), p. 6-9 (2008).

8. "Role of network connectivity in intercellular calcium signaling", I.V. Dokukina, M.E. Gracheva, E.A. Grachev and J.D. Gunton, *Physica D* **237**, p. 745-754 (2008).

9. "The influence of the tissue structure on intercellular calcium signaling", I.V. Dokukina, A.A. Tsukanov, M.E. Gracheva and E.A. Grachev, *Biophyzika* **53(2)**, p. 305-314 (2008) (in Russian).

10. "$p-n$ semiconductor membrane for electrically tunable ion current rectification and filtering", M.E. Gracheva, J. Vidal and J.-P. Leburton, *NanoLetters* **7**(6), p. 1717-1722 (2007). (This article was featured by: NSF.gov, Physicsdaily.com, IOP, Beckman Institute, NCSA, Electrical and computer engineering Department of UIUC and other sites internationally.)

11. "Electrolytic charge inversion at the liquid-solid interface in a nanopore in a doped semiconductor membrane", M.E. Gracheva and J.-P. Leburton, *Nanotechnology* **18**, p. 145704-145710 (2007).

12. "Electrically Tunable Solid-State Silicon Nanopore Ion Filter", J. Vidal, M.E. Gracheva and J.-P. Leburton, *Nanoscale Research Letters* **2**, p. 61-68 (2007).

13. "Modulation of mitochondrial calcium dynamics by cytosolic buffer proteins and cellular plasma membrane fluxes", I.V. Dokukina, M.E. Gracheva, E.A. Grachev, *Moscow State University Physics Bulletin* (Vestnik Moskovskogo Universiteta, Fizika) **2**, p. 23-26 (2007).

14. (Journal cover article) "Electrical Signatures of Single-Stranded DNA with Single Base Mutations in a Nanopore Capacitor", M.E. Gracheva, A. Aksimentiev and J.-P. Leburton, *Nanotechnology* **17(13)**, p. 3160-3165 (2006).

15. (The Most Accessed paper - top 10% of Institute of Physics (IOP) Publishing) "Simulation of the electric response of DNA translocation through a semiconductor nanopore-capacitor", M.E. Gracheva, A. Xiong, A. Aksimentiev, K. Schulten, G. Timp and J.-P. Leburton, *Nanotechnology* **17(3)**, p. 622-633 (2006).

16. "A finite-size scaling study of a model of globular proteins", D.L. Pagan, M.E. Gracheva and J.D. Gunton, *J. of Chem. Physics* **120(17)**, p. 8292-8298 (2004).

17. "A continuum model of motility in amoeboid cells", M.E. Gracheva and H.G. Othmer, *Bulletin of Math. Biology* **66(1)**, p. 167-193 (2004).

18. "The role of noise in some physical and biological systems", J.D. Gunton, R. Toral, C. Mirasso and M.E. Gracheva, chapter in book *"Recent Research Developments in Applied Physics"*, eds. M. Kawasaki, N. Ashgriz, R. Anthony (2003).

19. "Intercellular communication via intracellular calcium oscillations", M.E. Gracheva and J.D. Gunton, *J. of Theor. Biology* **221(4)**, p. 513-518 (2003).

20. "Stochastic simulation of intercellular calcium spiking in hepatocytes", M.E. Gracheva, R. Toral and J.D. Gunton, *J. Theor. Biology* **212**, p. 111-125 (2001).

21. "Coarse-grained Ginzburg-Landau free energy for Lennard-Jones systems", M.E. Gracheva, J.M. Rickman and J.D. Gunton, *J. Chem. Phys.* **113(9)**, p. 3525-3529 (2000).

22. "Phase transitions in a two-dimensional vortex system with defects: Monte Carlo simulation", V.A. Kashurnikov, I.A. Rudnev, M.E. Gracheva and O.A. Nikitenko, *J. of Exp. and Theor. Physics* **117**, p. 196 (2000).

23. "Phase transitions in a two-dimensional vortex lattice with defects: Monte Carlo simulation", I.A. Rudnev, V.A. Kashurnikov, M.E. Gracheva and O.A. Nikitenko, *Physica C* **332**, p. 383 (2000).

24. "Vortex lattice melting in layered HTSC in the field of defects", M.E. Gracheva, V.A. Kashurnikov, I.A. Rudnev and O.A. Nikitenko, *Low Temperature Physics* **25(10**, p.765 (1999).

25. "Dynamics of vortex lattice in the current state in high-temperature superconductors: Monte Carlo method", M.E. Gracheva, V.A. Kashurnikov, I.A. Rudnev, *Low Temperature Physics* **25(2)**, p.105 (1999).

26. "Phase diagram of layered HTSC: simulation by means of Monte Carlo method", M.E. Gracheva, V.A. Kashurnikov, I.A. Rudnev, *Physics of low-dimensional structures* **9/10**, p. 202-208 (1998).

27. "Monte Carlo simulation of phase transitions in the vortex system of high-temperature superconductors", M.E. Gracheva, M.V. Katargin, V.A. Kashurnikov and I.A. Rudnev, *Low Temperature Physics* **23(11)**, p.863 (1997).

28. "Features of the melting dynamics of a vortex lattice in a high-Tc superconductor in the presence of pinning centers", M.E. Gracheva, V.A. Kashurnikov and I.A. Rudnev, *J. of Exp. and Theor. Physics Letters* **66**, p.269-274, (1997).

29. "Monte-Carlo simulation of the two-dimensional vortex lattice melting in high-temperature superconductors with defects", M.E. Gracheva, V.A. Kashurnikov and I.A. Rudnev, *Physics of low-dimensional structures* **8/9**, p. 125-134 (1997).

In preparation:

1. "A simple model of DNA translocation through a nanopore", A. Nikolaev, M. Gracheva.

2. "Cell motility in tumor angiogenesis", N. Tarfulea, M. Gracheva and H. Othmer.

3. "Multi-point network method for spatially extended systems: application to calcium signaling", I. Dokukina, D. Melnikov, E. Grachev and M. Gracheva.

Invention disclosure/Patent: "Solid State Device: Molecular detection device", with Jean-Pierre Leburton, Gregory Timp and Julien Vidal, filed in May (2007), US Patent application #20090084688.

Grants:

1. USAR, Agency ID #W911NF-05-1-0339, Project Title: Smart Responsive nancomposites for soldier protection, sub-program: , Time Period: 06/12/2009-09/30/2011, Award amount $174,491.00 (0.3 share), PIs: Dan Goia, Vladimir Privman, Maria Gracheva.

2. National Center for Supercomputing Applications (UIUC), Grant TG-PHY070026N, "Application of layered semiconductor nanostructures for ion/bio-molecule filtering and characterization", August 1 (2008).

3. National Center for Supercomputing Applications (UIUC), Grant TG-PHY070026N, "Application of layered semiconductor nanostructures for ion/bio-molecule filtering and characterization", August 1 (2007).

Service:
Department of Physics, Open House, November 13th (2010)
NSF Panel, October 26th-27th, 2010
Department of Physics, Open House, October 2nd (2010)
Undergraduate student adviser (since 2008)

Reviewer for: IEEE Transactions on Electronic Devices (2010)
The Journal of Theoretical Biology (2008)
The Journal of Computational Electronics (2008, 2009)
IEEE Transaction on Nanotechnology (2009, 2010)
ACS Nano (2009)
The Journal of Chemical Physics (2009)
Langmuir (2009, 2010)
Physical Biology (2010)

Editor: of the book entitled "Nanopore-based technology: Single molecule characterization and DNA sequencing" (Publisher: Humana Press, Springer) which is scheduled to print in the early summer of 2010.

Membership: American Physical Society (since 2008), Biophysical Society (since 2008)

Honors: Listed in Who's Who in Science and Engineering, 10th Anniversary Edition, 2008-2009.
Best Paper Finalists, IEEE-NANO-2008, "Simulation of electrically tunable semiconductor nanopores for DNA sequencing", with J.-P. Leburton.

Highlights/News:

1. "Semiconductor membrane mimics biological behavior of ion channels", http://www.nsf.gov/news, http://www.physorg.com, Physicsdaily.com, Institute of Physics (IOP), Beckman Institute, NCSA, Electrical and Computer Engineering Department of UIUC and other sites internationally.

2. "Scientists tap NCSA resources to design a tunable semiconductor membrane that could be used for protein filtering or DNA sequencing", ACCESS journal, NCSA, vol. 20(3), Fall 2007.

3. Featured in "DNA Sequencing Using Nanopores Toward the Genomic Analysis of Cancer ", American Chemical Society, Chemistry Magazine, Autumn 2007.

Conferences and Seminars:

- (Invited talk) "Controlling DNA translocation through a semiconductor membrane", CECAM workshop on "Molecular simulation in external electric and electromagnetic fields", University College Dublin, Ireland, May 19th - May 21st (2011).
- (Invited seminar) SUNY Potsdam Spring 2011.
- (Poster) "Electrostatic trapping of polymers during translocation through a semiconductor nanopore", Biophysical Society Meeting, Baltimore, MD, March 5th - March 7th (2011).
- (Poster) "Simulation of ionic current through the nanopore in a double layered semiconductor membrane", Biophysical Society Meeting, Baltimore, MD, March 5th - March 7th (2011).
- (Invited seminar) "DNA sensing and characterization with a semiconductor nanopore, SUNY Binghamton University, October 18th (2010).
- (Freshman seminar) Single molecule sensing with a semiconductor nanopore, Clarskon University, September 6th (2010).
- (Invited talk) "The effect of the nanopore geometry on ionic currents in double layered semiconductor membranes", Summer School "Biosensing with channels", Berder Island, France, August 21th -August 27th (2010).
- (Invited talk) "A model of fibroblast rigidity sensing", AMS Meeting, Macalester College College, St. Paul MN, April 10th - April 11th (2010).
- (Poster) "Regulation of the ionic current flowing through a nanopore in a semiconductor membrane", Biophysical Society Meeting, San Francisco CA, February 20th - February 28th (2010).
- (Invited talk) "SPICE-circuit simualtion of the electrical response of a semiconductor membrane to a DNA molecule translocating through a nanopore", Nanoelectronic Devices for Defense & Security Conference (NANO-DDS), Fort Lauderdale FL, September 28th - October 2nd (2009).
- (Talk) "Computational model of controlled translocation of DNA molecule through a nanopore membrane with tunable electrostatic potential", American Physical Society, Pittsbugh PA, March 16th - March 20th (2009).
- (Talk) "Fibroblast motility on substrates with different rigidities: modeling approach", I. Dokukina and M. Gracheva, American Physical Society, Pittsbugh PA, March 16th - March 20th (2009).
- (Poster) "Computational model of controlled translocation of DNA molecule through a nanopore membrane with tunable electrostatic potential", Biophysicsl Society Meeting, Boston MA, February 28th - March 4th (2009).
- (Freshman Seminar) DNA detection and sequencing with a semiconductor nanopore, Department of Physics, Clarkson University, October 20 (2008).

- (Invited talk) 4th Special Workshop on Electronic Recognition of Bio-molecules, University of Liege, Belgium, September 10-12 (2008).
- (Invited talk) 15th International Conference on Superlattices, Nanostructures and Nanodevices (ICSNN 2008), Natal, Brazil, August 3-8 (2008).
- (Invited talk) "A model of fibroblast motility on substrates with different rigidities", American Mathematical Society conference, Indiana University, Bloomington Indiana, April 5-6 (2008).
- (Invited talk) "Protein and ion filtering with a semiconductor nanopore membranes", Nanohour, UIUC, February 13 (2008).
- "Protein and ion filtering with a semiconductor nanopore", NanoBio Seminar at University of Illinois at Urbana-Champaign, December 6 (2007).
- (Invited seminar) "Simulation of electrically tunable semiconductor nanopores for ion current/protein manipulation and DNA sequencing", Clarkson University, November 30 (2007).
- "Simulation of electrically tunable semiconductor nanopores for ion current/single bio-molecule manipulation", with Jean-Pierre Leburton, IWCE-12, University of Massachusetts, Amherst, October 8-10 (2007).
- (Invited talk, Best Paper Finalist) "Simulation of electrically tunable semiconductor nanopores for DNA sequencing", with Jean-Pierre Leburton, IEEE-NANO, Hong Kong, August (2007). UIUC ECE news hightlight: http://www.ece.uiuc.edu/news/.
- "Semiconductor membranes for ion current rectification and filtering", with Jean-Pierre Leburton, UIUC, Nanoscale Workshop Meeting, July 30-31 (2007).
- "Nanopore in a silicon membrane for ion current manipulation", NanoBio Seminar at University of Illinois at Urbana-Champaign, April 12 (2007).
- (Invited seminar) "DNA detection and sequencing with a semiconductor nanopore", Pennsylvania State University, September 18-20 (2006).
- (Invited talk) "Multi-grid method for DNA translocation through a semiconductor nanopore", with Jean-Pierre Leburton, ERBM-3, Belgium, September 6-8 (2006).
- "Topology of cellular networks in calcium signaling", with I. Dokukina and E.A. Grachev, p. 111 in Abstract Book, 9th European symposium on calcium-binding proteins in normal and transformed cells (9th European Calcium Society meeting), Strasbourg, France, 19-22 July 2006.
- "Decoding complex electrical signals produced by the DNA translocating through a solid state nanopore", 6th Understanding Complex Systems Symposium, dedicated to Paul C. Lauterbur, Nobel Prize in Physiology or Medicine, University of Illinois at Urbana-Champaign, May 15-18 (2006).
- "Electrical Signatures of Single-Stranded DNA in a Nanopore Capacitor: Single Base Mutations", with Jean-Pierre Leburton and A. Aksimentiev, MNTL/CNST Nanotechnology Workshop, Urbana-Champaign, Illinois, May 5-6 (2006).

- "Electrical response of DNA translocation through nanopore MOS-capacitor", with Jean-Pierre Leburton, A. Aksimentiev and G. Timp, MNTL/CNST Nanotechnology Workshop, Urbana-Champaign, Illinois, May 5-6 (2005).

- (Invited talk) "Self-consistent simulation of DNA translocation through an artificial nanopore", 2nd Conference on nanoscale devices and system integration, Houston, Texas, April 4-6 (2005).

- "Simulation of DNA translocation through a nanopore", with Jean-Pierre Leburton, ERBM-2, Beckman Institute, Urbana-Champaign, Illinois, September 7-9 (2005).

- "A Monte Carlo study of a model of globular protein nanoparticles", with D.L. Pagan and J.D. Gunton, NSTI Nanotechnology conference and trade show Nanotech 2004, Boston, Massachusetts, March 7-11 (2004).

- "Phase diagram for a model of globular proteins", D. Pagan, J.D. Gunton, M.E. Gracheva, American Physical Society (APS) Meeting, Austin, Texas (2003).

- "Modeling cell motility", M. E. Gracheva, H. G. Othmer, Gordon Research Conference in Theoretical Biology and Biomathematics, Tilton School, New Hampshire (2002).

- "Stochastic simulation of cell-cell signaling in hepatocytes", M. E. Gracheva, R. Toral, J. D. Gunton, First International Conference on Computational Nanoscience - ICCN 2001, Hilton Head Island, South Carolina (2001).

- "Intercellular calcium signaling via calcium receptor", M. E. Gracheva and J. D. Gunton, Symposium on Computational Cell Biology 2001: Lenox, Massachusetts (2001).

- "Numerical study of liquid-solid phase coexistence", M.E. Gracheva, J.M. Rickman, J.D. Gunton, American Physical Society (APS) Meeting, Minneapolis, Minnesota (2000).

- "Coarse-Grained Free Energy Functional for Lennard-Jones Systems", M.E. Gracheva, J.M. Rickman, J.D. Gunton, D.C. Coffey, Material Research Society (MRS) Symposium, Boston, Massachusetts (1999).

- "Self-organizing and disintegration of two-dimensional quasi-particles system in a trap", I.V. Voronin, M.E. Gracheva, E.Yu. Ul'ianov, in Proceedings of the International Conference of Graduate and Postgraduate Students "Lomonosov-98", Moscow State University, Moscow (1998).

- "Simulation of current-voltage characteristics of high-temperature superconductors with various types of defect structures", M.E. Gracheva, V.A. Kashurnikov, I.A. Rudnev, 5-th International Workshop on high-temperature superconductors and novel inorganic materials engineering; MSU-HTSC V (Moscow State University), abstract S-54 (1998).

- "Dynamics of vortex lattice with current in high temperature superconductors", M.E. Gracheva, V.A. Kashurnikov, I.A. Rudnev, Third Meeting on Low-Temperature Superconductivity, Moscow State University, Russia (1998).

- "Vortex lattice melting of HTSC in defect field", M.E. Gracheva, V.A. Kashurnikov, O.A. Nikitenko, I.A. Rudnev, Third Meeting on Low-Temperature Superconductivity, Moscow State University, Russia (1998).
- "Monte-Carlo simulation of vortex lattice in high-temperature superconductors", M.E. Gracheva, V.A. Kashurnikov, I.A. Rudnev, in Proceedings of the First Open Scientific Conference, Joint Institute for Nuclear Research, Dubna, Russia (1997).
- "Effect of defects configuration on vortex lattice in high-temperature superconductors", M.E. Gracheva, in Proceedings of the International Conference of Graduate and Postgraduate Students "Lomonosov-97", Moscow State University, Russia (1997).

Attended conferences:

- Annual teaching effectiveness conference sponsored by Associated Colleges: , St. Lawrence University, Canton, November , 2010.
- Annual teaching effectiveness conference sponsored by Associated Colleges: Teaching Digital Natives, Clarkson University, November 7th, 2009.
- Annual teaching effectiveness conference sponsored by Associated Colleges: Preparing our Students for the World through a Globalized Curriculum (Global Learning: Remapping the Curriculum), SUNY Canton, November 1st, 2008.

Undergraduate students supervised (past and present):
1) Suzanne Van Arsdale (spring 2009) Enzymatic chemical reactions.
2) Jeremiah M. Dederick (fall 2009) Electrostatic potential distribution in a nanoslit.
3) Padraic Cashin (fall 2009, spring 2010, summer 2010, fall 2010, summer 2011) Brownian dynamics model of DNA in a nano-slit.
4) Dmitry Bikulov (summer 2010, summer 2011) Brownian dynamics model of DNA in a nano-slit, cell biomechanics model.

Graduate students supervised (current):
Alexey Nikolaev (2008,2009,2010,2011)
George Nelson(2010,2011)

Post-doctoral researchers supervised (past and current):
Irina Dokukina (2008,2009)

Research with Summer graduate students and visitors:
Andrey Borunov (summer 2009)
Sergey Makarov (summer 2009, summer 2010)

References:

1. Professor Jean-Pierre P. Leburton
   Gregory Stillman Professor of Electrical and Computer Engineering
   Department of Electrical and Computer Engineering
   University of Illinois (Urbana-Champaign), IL
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2. Professor Gregory Timp
   Professor of Electrical and Computer Engineering
   Department of Electrical and Computer Engineering
   University of Illinois (Urbana-Champaign), IL
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   (217) 244-9629

3. Professor James D. Gunton
   Joseph A. Waldschmitt Professor of Physics
   Department of Physics
   Lehigh University, PA
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