

Denis O. Demchenko**Curriculum Vitae**

Physics Department
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EDUCATION:

- 2002 Ph.D., Department of Physics, South Dakota School of Mines & Technology, Rapid City, SD
Thesis Adviser: Prof. Andre G. Petukhov
Thesis Title: *Spin-Dependent Tunneling in Magnetic Heterostructures*
- 1996 M.S., Department of Physics, Division of Solid State Physics and Solid State Electronics, Odessa State University, Odessa, Ukraine

PROFESSIONAL AND RESEARCH EXPERIENCE:

- 2008-present: Assistant Professor, Physics Department, Virginia Commonwealth University, Richmond VA
- 2005-2008: Postdoctoral Research Fellow, Computational Nanoscience Group (Dr. Lin-Wang Wang), Computational Research Division, Lawrence Berkeley National Laboratory, Berkeley, CA
- 2002-2005: Postdoctoral Research Fellow, Condensed Matter Theory Group (Profs. Amy Y. Liu and J. K. Freericks), Department of Physics, Georgetown University, Washington, DC
- 1997-2002: Research Assistant, Solid State Theory Group (Prof. Andre G. Petukhov), Department of Physics, South Dakota School of Mines and Technology, Rapid City, SD

PROFESSIONAL AFFILIATIONS:

- American Physical Society
- Referee for: Physical Review Letters, Physical Review B, Europhysics Letters, Journal of Physics Chemistry, Journal of American Chemical Society, Central European Journal of Physics, Superlattices and Microstructures, ACS Applied Materials & Interfaces.
- Reviewer for research proposals for: NSF, Department of Energy INCITE program for large scale supercomputer allocations

RESEARCH:

- Theoretical calculations of point defect related luminescence in wide band gap semiconductors
- Theoretical methods of calculation of defect properties in semiconductors based on hybrid density functionals
- Defect complexes and carrier compensation mechanisms in wide band gap semiconductors
- Lattice thermal conductivity of complex metal oxides and their nanostructures
- Nanoscaling approaches to thermoelectricity by computing both lattice and electronic parts of thermal conductivity
- Molecular dynamics modeling of plasticity in nanowires and their strengthening mechanisms

PUBLICATIONS:

26. D. O. Demchenko, H.Y. Liu, V. Avrutin, N. Izyumskaya, Ü. Özgür, and H. Morkoç, “Binding of Ga complexes and self-compensation in Ga-doped ZnO”, submitted to *Journal of Applied Physics* (2013)
25. D. O. Demchenko and M. A. Reshchikov “Blue luminescence and Zn acceptor in GaN”, *Phys. Rev. B* **88**, 115204 (2013)
24. D. O. Demchenko and D. Ameen “Lattice thermal conductivity in bulk and nanosheet Na_xCoO_2 ”, submitted to *Computational Materials Science* (2013)
23. D. O. Demchenko, I. C. Diallo, and M. A. Reshchikov, “Yellow Luminescence of Gallium Nitride Generated by Carbon Defect Complexes”, *Phys. Rev. Lett.* **110**, 087404 (2013).
22. S. Curtarolo, W. Setyawana, G. L.W. Hart, M. Jahnatek, R. V. Chepulskii, R. H. Taylor, S. Wang, J. Xue, K. Yang, O. Levy, M. J. Mehl, H. T. Stokes, D. O. Demchenko, D. Morgan, “AFLOW: An automatic framework for high-throughput materials discovery” *Computational Materials Science* **58**, 218–226 (2012).
21. D. O Demchenko, P. D Heinz, B. H. Lee, “Determining factors of thermoelectric properties of semiconductor nanowires”, *Nanoscale Research Letters* **6**, 502 (2011).
20. D. O. Demchenko, B. Earles, H. Y. Liu, V. Avrutin, N. Izyumskaya, Ü. Özgür, and H. Morkoç, “Impurity complexes and conductivity of Ga-doped ZnO”, *Phys. Rev. B* **84**, 075201 (2011).
19. B. Sadtler, D. O. Demchenko, Haimei Zheng, S. M. Hughes, M. G. Merkle, U. Dahmen, Lin-Wang Wang, A. P. Alivisatos, “Selective facet reactivity during cation exchange in cadmium sulfide nanorods”, *J. Am. Chem. Soc.* **131**(14), 5285-5293 (2009).
18. D. O. Demchenko, S. G. Sacha, M. Salmeron, and Lin-Wang Wang, “Interactions of oxygen and hydrogen on Pd(111) surface”, *Surface Science*, **602**(14), 2552-2557 (2008).
17. D. O. Demchenko, R. D. Robinson, B. Sadtler, C. K. Erdonmez, A. P. Alivisatos, and Lin-Wang Wang, “Formation mechanism and properties of CdS-Ag₂S nanorod superlattices”, *ACS Nano*, **2**(4), 627-636 (2008).
16. D. O. Demchenko and Lin-Wang Wang, “Localized Electron States Near a Metal-Semiconductor Nanocontact”, *Nanoletters* **7**(10), 3219-3222 (2007).
15. J. Schrier, D. O. Demchenko, Lin-Wang Wang, A. P. Alivisatos, “Optical properties of ZnO/ZnS and ZnO/ZnTe heterostructures for photovoltaic applications”, *Nanoletters* **7**, 2377 (2007).
14. R. D. Robinson, B. Sadtler, D. O. Demchenko, C. K. Erdonmez, Lin-Wang Wang, A. P. Alivisatos, “Spontaneous Superlattice Formation in Nanorods through Partial Cation Exchange”, *Science* **317**, 355 (2007).
13. D. O. Demchenko and Lin-Wang Wang, “Optical transitions and nature of Stokes shift in spherical CdS quantum dots”, *Phys. Rev. B* **73**, 155326 (2006).
12. D. O. Demchenko and Amy Y. Liu, “Influence of interface structure on electronic properties and Schottky barriers in Fe/GaAs magnetic junctions”, *Phys. Rev. B*, **73**, 115332 (2006).
11. D. O. Demchenko, A. V. Joura, and J. K. Freericks, “Effect of Particle-Hole Asymmetry on the Mott-Hubbard Metal-Insulator Transition”, *Phys. Rev. Lett.* **92**, 216401 (2004).
10. D. O. Demchenko, Amy Y. Liu, E. Z. Kurmaev, L. D. Finkelstein, V. R. Galakhov, A. Moewes, S. G. Chiuzbaian, M. Neumann, C. R. Kmetz, K. L. Stevenson, “Electronic Structure of Transition Metal Dicyanamides $M[\text{N}(\text{CN})_2]_2$ ($M=\text{Mn, Fe, Co, Ni, Cu}$)”, *Phys. Rev. B* **69**, 205105 (2004).
9. A. V. Joura, D. O. Demchenko, and J. K. Freericks, “Thermal Transport in the Falicov-Kimball Model on a Bethe Lattice”, *Phys. Rev. B* **69**, 165105 (2004).
8. J. K. Freericks, D. O. Demchenko, A. V. Joura, and V. Zlatic, “Optimizing Thermal Transport in the Falicov-Kimball Model: Binary Alloy Picture”, *Phys. Rev. B* **68**, 195120 (2003).
7. A. G. Petukhov, D. O. Demchenko, and A. N. Chantis, “Electron Spin Polarization in Resonant Interband Tunneling Devices”, *Phys. Rev. B*, **68**, 125332 (2003).
6. A. G. Petukhov, A. N. Chantis, and D. O. Demchenko, “Resonant Enhancement of Tunneling Magnetoresistance in Double Barrier Heterostructures”, *Phys. Rev. Lett.* **89**, 107205, (2002).

5. D. O. Demchenko, A. N. Chantis, A. G. Petukhov, "Spin Filtering in Magnetic Heterostructures", *Internat. J. Modern. Phys. B* **15**, 3247 (2001).
4. A. G. Petukhov, D. O. Demchenko, A. N. Chantis, "Spin-Dependent Resonant Tunneling in Double Barrier Magnetic Heterostructures", *J. Vac. Sci. Technol. B* **18**, 2109 (2000).
3. D. P. Savin, Ya. O. Roizin, D. A. Demchenko, E. Mugenski, I. Sokolska, "Properties of Laser Ablated Porous Silicon", *Appl. Phys. Lett.* **69**, 3048 (1996).
2. A. N. Chantis, D. O. Demchenko, and A. G. Petukhov, "Spin-Valve Effect in Magnetic Resonant Tunneling Devices", *Mat. Res. Soc. Symp. Proc.* **690**, F7.4.1 (2002).
1. A. N. Chantis, D. O. Demchenko, A. G. Petukhov, and W. R. L. Lambrecht, "Electronic Structure of Tunable Materials MnAl and MnGa", *Mat. Res. Soc. Symp. Proc.* **603**, 207 (2000).

COMPUTING RESOURCE GRANTS:

- 2003 Principal Investigator (PI): "First-principles calculations of electronic properties of magnetic junctions", National Partnership for Advanced Computational Infrastructure (NPACI), awarded 72,000 hours on IBM (Power3) BlueHorizon at San Diego Supercomputer Center (SDSC), from 01 July 2003 to 30 June 2004.
- 2004 Principal Investigator (PI): "First-principles calculations of electronic properties of magnetic junctions: application for extension", NPACI, awarded 32,000 hours on IBM (Power4) DataStar at SDSC, from 01 July 2004 to 30 June 2005.

INVITED TALKS:

- *Effects of particle-hole asymmetry on the Mott-Hubbard metal-insulator transition*, APS March Meeting, Los Angeles CA, March 2005.
- *First principles study of electronic and transport properties of nanostructures*, University of Southern Mississippi, Hattiesburg MS, April 2005.
- *Electronic structure and Schottky barrier formation in Fe/GaAs magnetic junctions*, LBNL, Berkeley CA, May 2005.
- *Theory of semiconductor nanostructures: computation and experiment*, LBNL, Berkeley CA, May 2007.
- *Formation and properties of Ag₂S and Cu₂S nanorod heterostructures*, Case Western Reserve University, September 2009.
- *Nanorod heterostructures for photovoltaic applications*, Georgetown University, April 2010.
- *Hybrid Functional Calculations of Defect Properties in Wide Band Gap Semiconductors*, XXII International Materials Research Congress – Cancun, Mexico, August 2013.
- *Hybrid functional calculations of defect related optical properties in wide band gap semiconductors*, Energy, Materials, and Nanotechnology Conference – Chengdu, China, October 2013
- *Progress in computational approaches to defect physics in semiconductors*, International Conference on Small Science – Las Vegas NV, December 2013

CONTRIBUTED TALKS: (since joining VCU)

- Denis O. Demchenko, Bryce Sadtler, Haimei Zheng, A. Paul Alivisatos, and Lin-Wang Wang, "Morphology of Cu₂S-CdS and Ag₂S-CdS Nanorod Heterostructures", APS March Meeting, Pittsburgh PA, March 2009.
- Denis O. Demchenko, M. Salmeron, Lin-Wang Wang - "Interactions of oxygen and hydrogen on Pd(111) surface", APS March Meeting, Portland OR, March 2010
- Denis O. Demchenko, "Hybrid density functional study of gallium in ZnO", APS March Meeting, Dallas TX, March 2011

- Denis O. Demchenko, “Impurity complexes and conductivity of Ga-doped ZnO”, APS March Meeting, Boston MA, 2012
- Denis O. Demchenko, “Carbon Defect Complex as a Source of Yellow Luminescence in GaN”, APS March Meeting, Baltimore MD, March 2013
- Denis O. Demchenko, “Carbon Defect Complex as a Source of Yellow Luminescence in GaN”, 27th International Conference on Defects in Semiconductors – Bologna, Italy, July 2013

TEACHING:

2008-current Assistant Professor, Department of Physics, VCU
(average course/instructor evaluations: 3.9 – 4.1)

- University Physics I

Texts: *Physics for scientists and engineers*, R. D. Knight

- Modern Physics

Texts: *Modern Physics for Scientists and Engineers*, J.R. Taylor, C.D. Zafiratos, and M.A. Dubson

- Recitations* for University Physics I: Mechanics
- Recitations for University Physics II: Electricity and Magnetism

2003-2004 Teaching Assistant, Department of Physics, Georgetown University

- Tutorials* for non-science majors “Quantum World around Us”
Texts: *The Strange World of Quantum Mechanics*, Styer;
QED: The Strange Theory of Light and Matter, Feynmann;
The Quantum Universe, Hey and Walters
- Tutorials* for undergraduate Relativity and Quantum Mechanics
Texts: *Spacetime Physics*, Taylor and Wheeler;
An Introduction to Quantum Physics, French and Taylor

1998-2002 Teaching Assistant, Department of Physics, South Dakota School of Mines and Technology

- 1998-2002 Recitations for calculus based physics: Electricity and Magnetism
Texts: *Fundamentals of Physics*, Halliday & Resnick, *University Physics*, Benson
- 1999 Evaluation of student work for undergraduate Quantum Mechanics
Text: *Introduction to Quantum Mechanics*, Griffiths
- 1999-2002 Complete course (lectures, recitations, labs) of non-calculus based physics sequence: Electricity, Magnetism, Optics, and Relativity
Text: *Physics*, Cutnell and Johnson
- 2000 Guest-lecturing Solid State Physics
Text: *Solid State Physics*, Ashcroft & Mermin

1996/1997 Teaching assistant, Department of Physics, Odessa State University, Odessa, Ukraine

- Recitations for Thermodynamics and Statistical Physics
Text: *Statistical Physics*, Landau & Lifshitz

M.S. STUDENTS SUPERVISED

Ibrahima Diallo, MS Physics, (Spring 2013)

Alex Khammang, MS Physics, (Spring 2014)

*Note: During a tutorial and recitations as delivered at Georgetown and VCU, students work in small groups on worksheets that focus on important concepts and ideas. The instructors do not directly answer students’ questions, rather they help students to reason out the answers themselves.

SERVICE

Department:

- Physics Undergraduate Award Committee (2009 – present)
- Served on MS and Ph.D. degree committees
- Research advisor to undergraduate physics majors

College: College of Humanities and Science Library Committee representative from the Physics Department (2008 - present)

University: Goldwater Scholarship Committee (2009 - present)

OTHER SERVICE

- Served on NSF Panel in Computational and Data Driven Materials Research (March 2013)
- Served on NSF Panel in NSF Panel in Chemical Theory, Models and Computational Methods (March 2012)
- Served on NSF Panel in Materials World Network (March 2010)
- Regularly serve as NSF Mail in proposal reviewer