Curriculum Vitae for Andriy Zhugayevych

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Education

2007 Ph.D. in Solid State Physics, Department of Theoretical Physics, Institute of Physics (Kiev)
Thesis: Hopping transport and luminescence kinetics in nanostructured silicon
Advisor: Prof. I. Blonsky

1995 M.S. in Physics, Department of Theoretical Physics, Kiev State University (Ukraine)
Thesis: Classical fields in the gravitational field of a black hole
Advisor: Prof. P. Fomin
GPA: 4.93 out of 5

1990 High school diploma, Physics and Math Specialized School 145 (Kiev)

Employment

2014-pres. Assistant Professor at Skolkovo Institute of Science and Technology (Skoltech)
2011-2014 Postdoctoral Research Associate at Theoretical Division, Los Alamos National Laboratory
2008-2011 Postdoctoral Research Associate at Chemistry Department, University of Houston
2000-2007 Research Fellow at Department of Theoretical Physics, Institute of Physics (Kiev)
2000-2007 Assistant Professor at Department of Mathematics and Theoretical Radiophysics, Kiev State University

Research experience

2014-pres. Skolkovo Institute of Science and Technology,
Assistant Professor:

Materials Science – Electrochemical Energy Storage – Solid State Modeling

- Computational screening of metal-ion and metal-air batteries.

Materials Science – Organic Electronics – Molecular Modeling

- First-principles modeling of materials for organic electronics for their use in solar cells, light emitters, field-effect transistors. In particular, modeling of charge and exciton transport in π-conjugated systems including crystalline and amorphous solids and (bio)polymers.

2011-2014 Los Alamos National Laboratory, Theoretical Division,
Postdoctoral Research Associate, sponsors Dr. S. Tretiak and Dr. E. Batista:
Materials Science – Organic Electronics – Molecular Modeling

- Detailed theoretical characterization of crystallites of a molecular donor in a record-breaking organic photovoltaic device is performed and the factors improving power conversion efficiency are suggested (collaboration with CEEM DOE Energy Frontier Research Center in University of California at Santa Barbara).
- First-principles modeling of charge and exciton transport in organic molecular crystals is implemented as a computational toolbox allowing for comprehensive characterization of a molecular crystal (basic structural and electronic properties, molecular conformations, absorption/emission spectra, charge carrier mobility, exciton diffusion length etc.)
- Maple-based molecular modeling toolbox is developed largely simplifying the use of computational quantum chemistry (especially for beginners).
- Methods for solving Holstein-Peierls model, a commonly used model for the description of charge and energy transport in molecular solids are explored.

2008-2011 University of Houston, Chemistry Department,
Postdoctoral Research Associate, mentor Prof. V. Lubchenko:
Materials Science – Amorphous Inorganic Semiconductors – Theory

- Model for electronic midgap states in amorphous chalcogenide semiconductors is proposed explaining the observed anomalies in electronic properties of these materials.
- Ab-initio and semiempirical calculations of closed-shell interactions are performed elucidating the nature of noncovalent bonding in electron-rich solids and molecular clusters.
- Toolbox for solving and analyzing the 1D extended Hubbard-Peierls model, a keystone model featuring effects of electron-electron and electron-lattice interactions is implemented.
- Disordered Su-Schrieffer-Heeger model is explored simulating fluctuation-driven formation of structural pseudointerfaces hosting topologically-protected midgap electronic states in amorphous solids.

2000-2007 Kiev State University, Department of Mathematics and Theoretical Radiophysics,
Assistant Professor:
Mathematical Physics

- Efficient perturbation theory for a class of random matrices is developed using series rearrangement and partial summation techniques.
- Perturbation theory for operator semigroups is developed.
- Evaluation of Green's function for regular lattices (this function is routinely used in condensed matter theory) and general graphs, which is a tough computational problem, is implemented.

2000-2007 Institute of Physics, Department of Theoretical Physics,
Research Fellow:
Statistical Physics – Lattice Models

- Dynamic correlation function of a lattice gas is obtained in cluster expansion.
- Collective diffusion in a lattice gas with two coexisting phases is calculated.
- Low- and high-temperature, virial, and combined expansions for lattice gases are calculated.
- Various results for the random walk on a disordered lattice are obtained using perturbation theory, effective medium approximation, enumeration techniques etc.

2001-2006 Institute of Physics, Department of Theoretical Physics,
Research Assistant, mentor Prof. I. Blonsky (Department of Photonic Processes):
Materials Science – Nanostructured Semiconductors

- Anomalously slow decay of phosphorescence in porous silicon is explained.
- Method is developed for retrieving traps distribution from experimental data on phosphorescence kinetics in nanostructured silicon and some organic polymers.
- Simulation of charge carrier recombination in nano-Si in a model of localized states is implemented.
- Geometrical localization in bent undulating nanowires is investigated.

1995-1999 Institute of Physics, Department of Theoretical Physics,
Research Assistant, mentor Prof. B. Lev:
Statistical Physics

- Interaction mechanisms and pattern formation for particles in colloids and liquid crystals are considered.
- Phase diagram of a supersymmetric ideal Bose gas is calculated.

1994-1995 Kiev State University, Theoretical Physics Department,
Master's Thesis Research, mentor Prof. P. Fomin (Institute for Theoretical Physics):
Classical Field Theory – Black Holes

- No-hair theorem for black holes is extended to a general class of scalar fields.

1993 Kiev State University, Theoretical Physics Department,
Graduate study, mentor Prof. O. Pugach (Main Astronomical Observatory, Kiev):
Astrophysics – Variable Stars

- Light-curve of R CrB variables is reproduced in the model of expanding dust clouds.

1992 Kiev State University, Physics Department,
Undergraduate study, mentor Prof. O. Kalayda:

- Linear integral equations with general varying integration limits are studied.

1989-1990 Astronomical Observatory of Kiev State University,
High school student, mentor A. Tkachenko:
Observational Astronomy – Variable Stars

- Amateur variable star observer. As of 2005, submitted 293 observations to AAVSO.

Teaching experience

2014-pres. Assistant Professor at Skolkovo Institute of Science and Technology:

- **Computational Chemistry and Materials Modeling**
- **Survey of Materials**
- **Introduction to Maple**

2000-2007 Assistant at Kiev State University:

- **Symmetry Related Topics in Materials Science**: lecturer, 3 yr experience
- **Statistical Physics**: TA, 7 yr experience, developed lecture notes and problems book
- **Quantum Mechanics**: TA, 5 yr experience, developed lecture notes and problems book
- **Electrodynamics**: TA, 3 yr experience
- **Partial Differential Equations**: TA, 5 yr experience, published problems and solutions book
- **Ordinary Differential Equations**: TA, 5 yr experience, developed seminar notes
- **Calculus**: TA, 5 yr experience
- **Probability Theory**: TA, 1 yr experience

Professional activities

- ***Referee*** of: J Chem Phys, J Phys Chem C, J Phys Chem Lett, J Am Chem Soc, ACS Appl Mater Interfaces, Macromolecules, Comp Theor Chem, Phys Chem Chem Phys, RSC Advances, Nanoscale, Polym Chem, Mater Sci Eng B, Nat Comm, PLOS One, New J Chem
- Past ***Memberships***: American Physical Society, American Chemical Society, Ukrainian Physical Society, Soviet Union Astronomical Society (VAGO)
- Skoltech ***Service***: coordinator of educational program in Materials Science
- Kiev State University ***Service***: judging student competitions, recruiting new students
- Institute of Physics (Kiev) ***Service***: establishing Young Scientists Council

Skills

- Standard methods of theoretical physics at the level of Landau-Lifshitz course, basic methods of quantum field theory, most of the mathematical methods used in condensed matter theory.
- Computational quantum mechanics and statistical physics – experienced.
- Computational mathematics – routine use.
- Maple, Fortran, Python – experienced; C++, Mathematica, Matlab – basic knowledge.
- Fluent in Ukrainian, English, and Russian.

Grants and Fellowships

2016-2018	Co-PI	Volkswagen Grant “Understanding the dependence of charge transport on morphology in organic semiconductor films”
2016-2018	Co-Inv	RSF Grant “Design of advanced organic cathode materials for lithium and sodium batteries”
2015-2018	PI	CINT user project “Modeling of highly conducting undoped conjugated polymers”
2003-2004	Co-Inv	NATO Collaborative Linkage Grant “Fluctuations processes in particle migration on surfaces”
2001-2003	Co-Inv	Greek-Ukrainian Bilateral Collaboration Grant “Diffusion in the bulk and on surfaces of materials under strong particle interactions”
2001	PI	Ukrainian Fellowship for Young Scientists

Conferences organized

2013 Organic Solar Cells, Santa Fe, NM, May 6-9 (organizer)

List of Publications

Peer-reviewed publications

1. "Single crystal microwires of *p*-DTS(FBTTh$_2$)$_2$ and their use in the fabrication of field-effect transistors and photodetectors",
   Q Cui, Y Hu, C Zhou, F Teng, A Zhugayevych, S Tretiak, T-Q Nguyen, G C Bazan,
   submitted to *Adv. Func. Mater.* **2017**
2. "Crystal Structure and Li-Ion Transport in Li_2CoPO_4F High-Voltage Cathode Material for Li-Ion Batteries",
   S S Fedotov, A Kabanov, N Kabanova, V A Blatov, A Zhugayevych, A M Abakumov, N R Khasanova, E V Antipov,
   J. Phys. Chem. C **2017**, *121*, 3194 10.1021/acs.jpcc.6b11027
3. "Charge Delocalization Characteristics of Regioregular High Mobility Polymers",
   J. Coughlin, A. Zhugayevych, M. Wang, G. C. Bazan, S. Tretiak,
   Chem. Sci. **2017**, *8*, 1146 10.1039/C6SC01599A
4. "Modification of Optoelectronic Properties of Conjugated Oligomers Due to Donor/Acceptor Functionalization: DFT Study",
   A. Zhugayevych, O. Postupna, H.-L. Wang, S. Tretiak,
   Chem. Phys. **2016**, *481*, 133 10.1016/j.chemphys.2016.09.009
5. "Inter-aromatic distances in *Geobacter sulfurreducens* pili relevant to biofilm charge transport",
   H. Yan, C. Chuang, A. Zhugayevych, S. Tretiak, F. W. Dahlquist, G. C. Bazan,
   Adv. Mater. **2015**, *27*, 1908 10.1002/adma.201404167
6. "A new pH sensitive fluorescent and white light emissive material through controlled intermolecular charge transfer",
   Y. I. Park, O. Postupna, A. Zhugayevych, H. Shin, Y. S. Park, B. Kim, H.-J. Yen, P. Cheruku, J. S. Martinez, J. W. Park, S. Tretiak, H.-L. Wang,
   Chem. Sci. **2015**, *6*, 789 10.1039/c4sc01911c
7. "Polymorphism of crystalline molecular donors for solution-processed organic photovoltaics",
   T. S. van der Poll, A. Zhugayevych, E. Chertkov, R. C. Bakus II, J. E. Coughlin, G. C. Bazan, S. Tretiak, *J. Phys. Chem. Lett.* **2014**, *5*, 2700 10.1021/jz5012675
8. "A Combined Experimental and Theoretical Study of Conformational Preferences of Molecular Semiconductors",
   J. E. Coughlin, A. Zhugayevych, R. C. Bakus II, T. S. van der Poll, G. C. Welch, S. J. Teat, G. C. Bazan, S. Tretiak, *J. Phys. Chem. C* **2014**, *118*, 15610 10.1021/jp506172a
9. "Tailored electronic structure and optical properties of conjugated systems through aggregates and dipole-dipole interactions",
   Y. Park, C.-Y. Kuo, J. S. Martinez, Y.-S. Park, O. Postupna, A. Zhugayevych, S. Kim, J. Park, S. Tretiak, H.-L. Wang, *ACS Appl. Mater. Interfaces* **2013**, *5*, 4685 10.1021/am400766w
10. "Ab-initio study of a molecular crystal for photovoltaics: light absorption, exciton and charge carrier transport",
    A. Zhugayevych, O. Postupna, R. C. Bakus II, G. C. Welch, G. C. Bazan, S. Tretiak,
    J. Phys. Chem. C **2013**, *117*, 4920 10.1021/jp310855p

11. “Electronic structure and the glass transition in pnictide and chalcogenide semiconductor alloys. II. The intrinsic electronic midgap states”,
A. Zhugayevych, V. Lubchenko,
J. Chem. Phys. **2010**, *133*, 234504; arXiv: 1006.0776 10.1063/1.3511708
12. “Electronic structure and the glass transition in pnictide and chalcogenide semiconductor alloys. I. The formation of the ppσ-network”,
A. Zhugayevych, V. Lubchenko,
J. Chem. Phys. **2010**, *133*, 234503; arXiv: 1006.0771 10.1063/1.3511707
13. “An intrinsic formation mechanism for midgap electronic states in semiconductor glasses”,
A. Zhugayevych, V. Lubchenko, *J. Chem. Phys.* **2010**, *132*, 044508 10.1063/1.3298989
14. “Dynamic correlations in an ordered c(2×2) lattice gas”,
P. Argyrakis, M. Maragakis, O. Chumak, A. Zhugayevych, *Phys. Rev. B* **2006**, *74*, 035418
15. “Charge pump effect and mechanisms of charge carriers localization in oxidized nano-Si”,
I. V. Blonskyy, V. Kadan, A. Kadashchuk, A. Vakhnin, A. Zhugayevych,
Int. J. Nanotechnology **2006**, *3*, 65
16. “Approximate calculation of operator semigroups by perturbation of generators”,
A. Yurachkivsky, A. Zhugayevych, *Reports Nat. Acad. Sci. Ukraine* **2003**, *11*, 27
17. “New mechanism of charge carriers localization in silicon nanowires”,
I. V. Blonskyy, V. Kadan, A. Kadashchuk, A. Vakhnin, A. Zhugayevych, I. Chervak,
Physics of Low-Dimensional Structures **2003**, *7/8*, 25
18. “Influence of structural inhomogeneity on the luminescence properties of silicon nanocrystallites”,
I. V. Blonskii, M. S. Brodyn, A. Vakhnin, A. Zhugayevych, V. Kadan, A. Kadashchuk,
Low Temperature Physics **2002**, *28*, 706
19. “Locality of the Green function of kinetic equation on a lattice”,
A. Zhugayevych, *Bull. Univ. Kiev (Ser. fiz.-mat. nauky)* **2002**, *2*, 401, in ukrainian
20. “On linear integral equations with varying integration limits”,
O. F. Kalayda, A. Zhugayevych, T. Skrypnyk, *Bull. Univ. Kiev* **1999**, *4*, 33, in ukrainian
21. “Statistical description of model systems of interacting particles and phase transitions accompanied by cluster formation”,
B. I. Lev, A. Zhugaevych, *Phys. Rev. E* **1998**, *57*, 6460

Other publications

22. “Theoretical Description of Structural and Electronic Properties of Organic Photovoltaic Materials”,
A. Zhugayevych, S. Tretiak,
Ann. Rev. Phys. Chem. **2015**, *66*, 305 10.1146/annurev-physchem-040214-121440
23. “Mathematical physics in problems and solutions”,
A. Yurachkivsky, A. Zhugayevych, (Kiev Univ., **2005**), 158 pages, in ukrainian
24. “DNA, DNA/metal nanoparticles, DNA/nanocarbon and macrocyclic metal complexes/fullerene molecular building blocks for nanosystems: Electronics and sensing”,
E. Buzaneva, A. Gorchinskiy, P. Scharff, P. Risch, A. Nassiopoulou, C. Tsamis, Yu. Prilutskyy, O. Ivanyuta, A. Zhugayevych, D. Kolomiyets, A. Veligura, I. Lysko, O. Vysokolyan, O. Lysko,

D. Zherebetskyy, A. Khomenko, I. Sporysh, in *Frontiers of Multifunctional Integrated Nanosystems*, ed. E. Buzaneva, P. Scharff, p. 251 (Kluwer, **2004**)

Invited presentations

25. "First-principle modeling of energy and charge transport in organic semiconductors", *3rd International Fall School on Organic Electronics* (Moscow, **2016**)
26. "First-principle effective Hamiltonian modeling of charge and energy transfer in molecular systems: Picosecond-scale phenomena", *Mesilla Chemistry Workshop "Electrochemical Processes: Photovoltaics and Charge Transfer in Nanomaterials"* (Mesilla, NM, **2016**); talk
27. "First principle modeling of materials for organic electronics", *Institute of Physics, Department of Theoretical Physics Colloquium* (Kiev, **2014**)
28. "Multiscale modeling of nanomaterials with application to organic solar cells", *Massachusetts Institute of Technology, MIT Skoltech Initiative* (Boston, MA, **2014**)
29. "Ultrafast exciton dissociation in small-molecule bulk-heterojunction solar cells", *Telluride conference on Advances in Photoreactions* (Telluride, CO, **2013**)
30. "Midgap electronic states in amorphous pnictide and chalcogenide semiconductors", *LANL Center for Integrated Nanotechnologies Colloquium* (Los Alamos, NM, **2011**)

Contributed presentations (English-language presenter only)

31. "Towards rational design of organic solar cells: How to control the structure of a bulk material", *Atomistic Simulation of Functional Materials* (Moscow, **2014**); talk
32. "Exciton transport in a crystal of "soft" molecules beyond small polaron hopping", *Excited State Processes* (Santa Fe, NM, **2014**); poster
33. "Multiscale modeling of exciton and charge carrier transport in organic semiconductors", *Organic Solar Cells* (Sante Fe, NM, **2013**); talk
34. "First principles modeling of donor materials for organic solar cells: where theory complements experiment", *APS March Meeting* (Baltimore, MD, **2013**); talk
35. "First-principles modeling of exciton and charge transport in organic semiconductors: dependence on quantum chemistry method", *ACS Fall Meeting* (Philadelphia, PA, **2012**); poster
36. "First-principles study of exciton and charge transport in molecular crystals of dithienosilole-pyridylthiadiazole family: dependence on chemical composition", *Int. Conference on Science and Technology of Synthetic Metals* (Atlanta, GA, **2012**); poster
37. "First-principles study of energy and charge transport in molecular donors for organic solar cells", A. Zhugayevych, E. Batista, S. Tretiak, *LANL Postdoc Research Day* (Los Alamos, NM, **2012**); poster
38. "Understanding the high device efficiency of a class of solution-processed small-molecule solar cells", A. Zhugayevych, O. Postupna, S. Tretiak, G. C. Bazan, *APS March Meeting* (Boston, MA, **2012**); talk.

39. “Charge carrier transport in pi-conjugated systems: stacks versus polymers”, *XXVII Southwest Theoretical Chemistry Conference* (Lubbock, TX, **2011**); poster
40. “What determines the charge state of a soliton in conjugated polymers?”, *Int. Conference "Optical Probes of Conjugated Polymers"* (Santa Fe, NM, **2011**); poster
41. “An intrinsic formation mechanism for midgap electronic states in semiconductor glasses”, *XXV Southwest Theoretical Chemistry Conference* (Houston, TX, **2009**); poster
42. “Efficient perturbation expansion for disordered systems”, *III International Conference "Electronics and Applied Physics"* (Kiev, Ukraine, **2007**); talk
43. “Longtime asymptotics of porous silicon photoluminescence decay”, *International Young Scientists Conference on Applied Physics* (Kiev, **2001**); talk
44. “Long-time asymptotics of the photoluminescence decay: the role of diffusion and disorder”, *NATO/EC Workshop "Frontiers of nano-optoelectronic system"* (Kiev, **2000**); talk
45. “Hopping transport in nanocrystallites structures”, *International Conference "Advanced Materials"* (Kiev, **1999**); poster
46. “Hopping transport and photoluminescence in nanocrystallites structures”, *Physical Problems in Material Science of Semiconductors* (Chernivtsi, Ukraine, **1999**); talk