Curriculum Vitae for Andriy Zhugayevych

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Polymer Theory Department
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Education

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

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

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

Employment

2022 Visiting Researcher at Max Planck Institute for Polymer Research (MPIP)
2014-2022 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 (Kyiv)
2000-2007 Assistant at Department of Mathematics and Theoretical Radiophys., Kyiv State University

Research interests and expertise

- Computational materials science: molecules and solids, multiscale and high-throughput modeling, charge and energy transport
- Organic electronics
- Energy storage and conversion: batteries, solar cells
- Mathematical and theoretical physics and chemistry: lattice models

Most important results

- **Organic semiconductors**: contributed to development of first principle multiscale modeling of these materials solving several puzzles on their molecular and electronic structure.
- **Inorganic semiconductors**: discovered polarons in pnictogens; provided a unified picture of pnictides and chalcogenides as ppσ-networks; developed a methodology for reconstruction of electronic traps distribution from experimental data on phosphorescence kinetics.
- **Theoretical physics**: using lattice gas model demonstrated how to construct virial expansion for dynamic correlation function.

See research highlights web-page at http://zhugayevych.me/research

Research experience

2014-2022 Assistant Professor at Skolkovo Institute of Science and Technology:
Computational Materials Science – Organic Semiconductors

- First-principles modeling of materials for organic electronics for their use in solar cells, light emitters, field-effect transistors as well as for energy storage.

Computational Materials Science – Electrochemical Energy Storage

- Computational screening of metal-ion batteries: electrodes, membranes.

2011-2014 Postdoc at Los Alamos National Laboratory, mentors S. Tretiak and E. Batista:
Computational Materials Science – Organic Electronics

- First-principles modeling of organic solar cells and light emitters (collaboration with CEEM DOE Energy Frontier Research Center in University of California at Santa Barbara).

2008-2011 Postdoc at University of Houston, Chemistry Department, mentor V. Lubchenko:
Theoretical Materials Science – Amorphous Inorganic Semiconductors

- Model for electronic midgap states in amorphous chalcogenide semiconductors is developed explaining the observed anomalies in electronic properties of these materials.

2000-2007 Assistant at Dep. of Mathematics and Theoretical Radiophysics, Kyiv State University:
Mathematical Physics – Models of Disorder

- Various results for the random walk on a disordered lattice are obtained using perturbation theory, effective medium approximation, enumeration techniques etc.

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

- Dynamic correlation function of a lattice gas is obtained in cluster expansion.

Theoretical 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.

1995-1999 PhD student at Institute of Physics, Department of Theoretical Physics, mentor B. Lev:
Statistical Physics – Continuous Models

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

1990-1995 BSc student at Kyiv State University, Theoretical Physics Department:
Classical Field Theory, Astrophysics, Mathematical Physics

- No-hair theorem for black holes is generalized to a class of scalar fields (mentor P. Fomin).
- Light-curve of R CrB variables is modeled by expanding dust clouds (mentor O. Pugach).
- Linear integral equations with varying integration limits are studied (mentor O. Kalayda).

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

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

Teaching experience

2014-2022 Assistant Professor at Skolkovo Institute of Science and Technology:

- **Computational Chemistry and Materials Modeling**: instructor, 8 yr experience
- **Survey of Materials**: instructor, 6 yr experience
- **Advanced Materials Modeling**: lecturer, 3 yr experience
- **Organic Materials for Energy and Optoelectronics**: instructor, 1 yr experience
- **Introduction to Maple**: instructor, 1 yr experience

2000-2007 Assistant at Kyiv State University:

- **Symmetry Related Topics in Materials Science**: instructor, 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/solutions book
- **Ordinary Differential Equations**: TA, 5 yr experience, developed seminar notes
- **Calculus**: TA, 5 yr experience
- **Probability Theory**: TA, 1 yr experience

Mentoring

- ***Graduated MSc students***: 5 in computational and experimental materials science
- ***Postdocs***: Dmitry Aksenov, Nikita Tukachev
- ***Research interns*** (short- or part-time appointments): 4 in computational materials science
- ***Individual Doctoral Committee*** member for more than 10 PhD students in materials science
- For hundreds of students I taught at least 3 different courses (>10 contact hours per student)

See alumni web-page at http://zhugayevych.me/alumni.htm

Professional activities

- ***Referee*** of 25 journals of 7 publishers: **ACS** – J Phys Chem C, J Phys Chem Lett, J Chem Theory Comp, J Am Chem Soc, Nano Lett, ACS Appl Mater Interfaces, Macromolecules; **RSC** – Phys Chem Chem Phys, RSC Advances, Nanoscale, Polym Chem, J Mater Chem C, New J Chem; **Springer** – Nat Comm, Sci Rep, Theor Chem Acc; **Wiley** – Adv Theor Simul, Adv Mater, Adv Electron Mater, Int J Quant Chem; **Elsevier** – Comp Theor Chem, Mater Sci Eng B, Dyes Pigm; **AIP** – J Chem Phys; **PLOS** – PLOS One
- Skoltech ***MSc/PhD Defense*** Committee member: 1-2 times per year in 2017-2021
- Skoltech ***Service***: coordinator of Computational Materials Science Laboratory
- Skoltech ***Service***: coordinator of educational program in Materials Science
- Skoltech ***Service***: coordinator of entry math exam for several programs (2017-18,2020-21)
- Kyiv State University ***Service***: judging student competitions, recruiting new students
- Institute of Physics (Kyiv) ***Service***: establishing Young Scientists Council
- Past ***Memberships***: American Physical Society, American Chemical Society, Ukrainian Physical Society, Soviet Union Astronomical Society (VAGO)

Skills

- Standard methods of theoretical physics at the level of Landau-Lifshitz course, basic methods of quantum field theory, most of the mathematical and computational methods used in condensed matter theory and materials science.
- Computational materials science – experienced.
- Computational mathematics – routine use.
- Maple, Fortran, Python – experienced; other computer languages – per-demand use.
- Fluent in Ukrainian, English, and Russian.

Grants and Fellowships

2020-2021	PI	CINT user project “Modeling of charge transport in solids of large molecules”, 2019BC0120
2018-2020	Co-Inv	RSF Grant “Spectroscopic method for evaluation of charge mobility in organic semiconductors”, 18-72-10165
2017-2019	Co-Inv	Next Generation Program: Skoltech-MIT joint project “Lithium redox flow batteries for high power and high energy density energy storage”
2016-2020	Co-Inv	RSF Grant “Design of advanced organic cathode materials for lithium and sodium batteries”, 16-13-00111
2016-2020	Co-PI	Volkswagen Grant “Understanding the dependence of charge transport on morphology in organic semiconductor films”, A115678
2015-2019	PI	CINT user project “Modeling of highly conducting undoped conjugated polymers”, U2015A0016, 2016BC0035, 2018AC0081
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)

Professional References

Prof. Sergei Tretiak
Theoretical Division
Los Alamos National Laboratory
Los Alamos, NM 87545, USA
serg@lanl.gov, +15056678351

Prof. Keith Stevenson
Center for Energy Science and Technology
Skolkovo Institute of Science and Technology
Moscow 121205, Russia
k.stevenson@skoltech.ru, +74952801481ext3373

Prof. Vassiliy Lubchenko
Chemistry Department
University of Houston
Houston, TX 77204, USA
vas@uh.edu, +18328428853

Prof. Ivan Blonskyi
Laser Femtosecond Complex
Institute of Physics
Kyiv 03028, Ukraine
blon@iop.kiev.ua, +380445259810

List of Publications

Google Scholar profile: *700 citations, h-index 15, h5-index 14, i10-index 21*
Scopus/WoS h-index is 14/15; SciVal FWCI 2015-2021 is 1.51 (1.69 for Materials Science)

Peer-reviewed publications

1. Single-particle and collective excitations of polar water molecules confined in nano-pores within a cordierite crystal lattice,
   M Belyanchikov, Z Bedran, M Savinov, P Bednyakov, P Proschek, J Prokleska, V Abalmasov, E Zhukova, V Thomas, A Dudka, **A Zhugayevych**, J Petzelt, A Prokhorov, V Anzin, R Kremer, J Fischer, P Lunkenheimer, A Loidl, E Uykur, M Dressel, B Gorshunov,
   Phys Chem Chem Phys 24, 6890 (**2022**) 10.1039/d1cp05338h IF2020=3.7, Q1
2. Small Polarons in Two-Dimensional Pnictogens: A First-Principles Study,
   V Vasilchenko, S Levchenko, V Perebeinos, **A Zhugayevych**,
   J Phys Chem Lett 12, 4674 (**2021**) 10.1021/acs.jpclett.1c00929 IF2019=6.7, Q1,NI
3. Hydroxyl Defects in LiFePO4 Cathode Material: DFT+U and an Experimental Study,
   D Aksyonov, I Varlamova, I Trussov, A Savina, A Senyshyn, K Stevenson, A Abakumov, **A Zhugayevych**, S Fedotov,
   Inorg Chem 60, 5497 (**2021**) 10.1021/acs.inorgchem.0c03241 IF2019=4.8, Q1,NI
4. Microcrystal Electron Diffraction for Molecular Design of Functional Non-Fullerene Acceptor Structures,
   S Halaby, M W Martynowycz, Z Zhu, S Tretiak, **A Zhugayevych**, T Gonen, M Seifrid,
   Chem Mater 33, 966 (**2021**) 10.1021/acs.chemmater.0c04111 IF2019=9.6, Q1
5. Impact of the acceptor units on optoelectronic and photovoltaic properties of (XDADAD)n-type copolymers: Computational and experimental study,
   I V Klimovich, F A Prudnov, O Mazaleva, N V Tukachev, A V Akkuratov, I V Martynov, A S Peregudov, A F Shestakov, **A Zhugayevych**, P A Troshin,
   Dyes and Pigments 185, 108899 (**2021**) 10.1016/j.dyepig.2020.108899 IF2019=4.6, Q1
6. Reversible electrochemical potassium deintercalation from >4 V positive electrode material K6(VO)2(V2O3)2(PO4)4(P2O7),
   I V Tereshchenko, D A Aksyonov, **A Zhugayevych**, E V Antipov, A M Abakumov,
   Solid State Ionics 357, 115468 (**2020**) 10.1016/j.ssi.2020.115468 IF2019=3.1, Q1
7. Dielectric ordering of water molecules arranged in a dipolar lattice,
   M A Belyanchikov, M Savinov, Z V Bedran, P Bednyakov, P Proschek, J Prokleska, V A Abalmasov, J Petzelt, E S Zhukova, V G Thomas, A Dudka, **A Zhugayevych**, A S Prokhorov, V B Anzin, R K Kremer, J K H Fischer, P Lunkenheimer, A Loidl, E Uykur, M Dressel, B Gorshunov,
   Nat Commun 11, 3927 (**2020**) 10.1038/s41467-020-17832-y IF2019=12, Q1,NI
8. Design of novel thiazolothiazole-containing conjugated polymers for organic solar cells and modules,
   A Akkuratov, S Nikitenko, A Kozlov, P Kuznetsov, I Martynov, N Tukachev, **A Zhugayevych**, I Visoly-Fisher, E Katz, P Troshin,
   Solar Energy 198, 605 (**2020**) 10.1016/j.solener.2020.01.087 IF2018=4.7, Q1

9. Correlating structure and transport properties in pristine and environmentally-aged superionic conductors based on Li1.3Al0.3Ti1.7(PO4)3 ceramics,
M Pogosova, I Krasnikova, A Sergeev, **A Zhugayevych**, K Stevenson,
J Power Sources 448, 227367 (**2020**) 10.1016/j.jpowsour.2019.227367 IF2018=7.5, Q1

10. Effects of pi-spacer and fluorine loading on the optoelectronic and photovoltaic properties of (X-DADAD)n benzodithiophene-based conjugated polymers,
A V Akkuratov, I E Kuznetsov, P M Kuznetsov, N V Tukachev, I V Martynov, S L Nikitenko, A V Novikov, A V Chernyak, **A Zhugayevych**, P A Troshin,
Synthetic Metals 259, 116231 (**2020**) 10.1016/j.synthmet.2019.116231 IF2018=2.9, Q2

11. Tuning optical properties of conjugated molecules by Lewis acids: insights from electronic structure modeling,
H Phan, T J Kelly, **A Zhugayevych**, G C Bazan, T Q Nguyen, E A Jarvis, S Tretiak,
J Phys Chem Lett 10, 4632 (**2019**) 10.1021/acs.jpclett.9b01572 IF2017=8.7, Q1,NI

12. Ground state geometry and vibrations of polyphenylenevinylene oligomers,
N V Tukachev, D R Maslennikov, A Y Sosorev, S Tretiak, **A Zhugayevych**,
J Phys Chem Lett 10, 3232 (**2019**) 10.1021/acs.jpclett.9b01200 IF2017=8.7, Q1,NI

13. Understanding migration barriers for monovalent ion insertion in transition metal oxide and phosphate based cathode materials: A DFT study,
D A Aksyonov, S S Fedotov, K J Stevenson, **A Zhugayevych**,
Comp Mater Sci 154, 449 (**2018**) 10.1016/j.commatsci.2018.07.057 IF2017=2.5, Q1

14. Reversible facile Rb+ and K+ ions de/insertion in a KTiOPO4-type RbVPO4F cathode material,
S S Fedotov, A S Samarin, V Nikitina, D Aksyonov, S Sokolov, **A Zhugayevych**, K Stevenson, N R Khasanova, A Abakumov, E V Antipov,
J Mater Chem A 6, 14420 (**2018**) 10.1039/C8TA03839B IF2017=9.9, Q1

15. Lowest-energy crystalline polymorphs of P3HT,
A Zhugayevych, O Mazaleva, A Naumov, S Tretiak,
J Phys Chem C 122, 9141 (**2018**) 10.1021/acs.jpcc.7b11271 IF2016=4.5, Q1

16. The role of semilabile oxygen atoms for intercalation chemistry of the metal-ion battery polyanion cathodes,
I V Tereshchenko, D A Aksyonov, O A Drozhzhin, I A Presniakov, A V Sobolev, **A Zhugayevych**, D Striukov, K J Stevenson, E Antipov, A M Abakumov,
J Am Chem Soc 140, 3994 (**2018**) 10.1021/jacs.7b12644 IF2016=14, Q1,NI

17. 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, J Huang, **A Zhugayevych**, S Tretiak, T-Q Nguyen, G C Bazan,
Adv Func Mater 28, 1702073 (**2018**) 10.1002/adfm.201702073 IF2016=12, Q1,NI

18. Vibrational states of nano-confined water molecules in beryl investigated by first-principles calculations and optical experiments,
M A Belyanchikov, E S Zhukova, S Tretiak, **A Zhugayevych**, M Dressel, F Uhlig, J Smiatek, M Fyta, V G Thomas, B P Gorshunov,
Phys Chem Chem Phys 19, 30740 (**2017**) 10.1039/C7CP06472A IF2016=4.1, Q1

19. 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 121, 3194 (**2017**) 10.1021/acs.jpcc.6b11027 IF2016=4.5, Q1

20. Charge delocalization characteristics of regioregular high mobility polymers,
J Coughlin, **A Zhugayevych**, M Wang, G C Bazan, S Tretiak,
Chem Sci 8, 1146 (**2017**) 10.1039/C6SC01599A IF2016=8.7, Q1,NI

21. 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 481, 133 (**2016**) 10.1016/j.chemphys.2016.09.009 IF2016=1.8, Q2

22. Theoretical description of structural and electronic properties of organic photovoltaic materials,
A Zhugayevych, S Tretiak,
Annu Rev Phys Chem 66, 305 (**2015**)10.1146/annurev-physchem-040214-121440,IF2016=15,Q1

23. 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 27, 1908 (**2015**) 10.1002/adma.201404167 IF2016=20, Q1,NI

24. 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 6, 789 (**2015**) 10.1039/c4sc01911c IF2016=8.7, Q1,NI

25. 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 5, 2700 (**2014**) 10.1021/jz5012675 IF2016=9.4, Q1

26. 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 118, 15610 (**2014**) 10.1021/jp506172a IF2016=4.5, Q1

27. 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 5, 4685 (**2013**) 10.1021/am400766w IF2013=7.5, Q1

28. 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 117, 4920 (**2013**) 10.1021/jp310855p IF2013=4.8, Q1

29. 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 133, 234504 (**2010**); arXiv: 1006.0776 10.1063/1.3511708 IF2010=2.9, Q1

30. 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 133, 234503 (**2010**); arXiv: 1006.0771 10.1063/1.3511707 IF2010=2.9, Q1

31. An intrinsic formation mechanism for midgap electronic states in semiconductor glasses,
A Zhugayevych, V Lubchenko,
J Chem Phys 132, 044508 (**2010**) 10.1063/1.3298989 IF2010=2.9, Q1

32. Dynamic correlations in an ordered c(2×2) lattice gas,
P Argyrakis, M Maragakis, O Chumak, **A Zhugayevych**,
Phys Rev B 74, 035418 (**2006**) 10.1103/PhysRevB.74.035418 IF2008=3.3, Q1

33. 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 3, 65 (**2006**) 10.1504/IJNT.2006.008721 Q2

34. Approximate calculation of operator semigroups by perturbation of generators,
A Yurachkivsky, A Zhugayevych, *Reports Nat Acad Sci Ukraine* 11, 27 (**2003**)

35. 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 7/8, 25 (**2003**)

36. 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 28, 706 (**2002**)

37. Locality of the Green function of kinetic equation on a lattice,
A Zhugayevych, *Bull Univ Kyiv (Ser fiz-mat nauky)* 2, 401 (**2002**), in ukrainian

38. On linear integral equations with varying integration limits,
O F Kalayda, **A Zhugayevych**, T Skrypnyk, *Bull Univ Kyiv* 4, 33 (**1999**), in ukrainian

Other publications

39. Broad-Band Spectroscopy of Nanoconfined Water Molecules,
M. A. Belyanchikov, M. Savinov, Z. V. Bedran, P. Bednyakov, P. Proschek, J. Prokleska, V. I. Torgashev, E. S. Zhukova, S. S. Zhukov, L. S. Kadyrov, V. Thomas, A. Dudka, **A. Zhugayevych**, V. B. Anzin, R. K. Kremer, J. K. H. Fischer, P. Lunkenheimer, A. Loidl, E. Uykur, M. Dressel, B. Gorshunov, in *4th International Conference on Nanotechnologies and Biomedical Engineering*, ed I. Tiginyanu et al., p.7 (Springer, **2020**)
10.1007/978-3-030-31866-6_2

40. Mathematical physics in problems and solutions,
A. Yurachkivsky, **A. Zhugayevych**, (Kyiv Univ., **2005**), 158 pages, in ukrainian

41. 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

42. Computational studies of organic semiconductors,
1st International School on Hybrid, Organic and Perovskite Photovoltaics (Moscow, **2019**)
43. Modeling of electronic properties of organic semiconductors,
Inaugural Symposium for Computational Materials Program of Excellence (Moscow, **2019**)
44. Modeling of charge transport in materials for energy and optoelectronics,
LANL Center for Nonlinear Studies Colloquium (Los Alamos, NM, **2017**)
45. Modeling of conjugated polymers: non-oligomer approach,
Telluride workshop Nonequilibrium Phenomena, Nonadiabatic Dynamics and Spectroscopy (Telluride, CO, **2017**)
46. First-principle modeling of energy and charge transport in organic semiconductors,
3rd International Fall School on Organic Electronics (Moscow, **2016**)
47. 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**)
48. First principle modeling of materials for organic electronics,
Institute of Physics, Department of Theoretical Physics Colloquium (Kyiv, **2014**)
49. Multiscale modeling of nanomaterials with application to organic solar cells,
Massachusetts Institute of Technology, MIT Skoltech Initiative (Boston, MA, **2014**)
50. Ultrafast exciton dissociation in small-molecule bulk-heterojunction solar cells,
Telluride conference on Advances in Photoreactions (Telluride, CO, **2013**)
51. 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)

52. Comparison of non-fullerene acceptors: How geometry influences electronic transport,
2nd International School on Hybrid, Organic and Perovskite Photovoltaics (Moscow, **2020**)
53. Polymorphism and charge transport in organic semiconductors,
4th International Fall School on Organic Electronics (Moscow, **2018**); talk
54. Challenges in Computational Design of Organic Semiconductors,
14th International Conference on Organic Electronics (Bordeaux, **2018**); poster
55. Towards rational design of organic solar cells: How to control the structure of a bulk material,
Atomistic Simulation of Functional Materials (Moscow, **2014**); talk

56. Exciton transport in a crystal of soft molecules beyond small polaron hopping,
Excited State Processes (Santa Fe, NM, **2014**); poster
57. Multiscale modeling of exciton and charge carrier transport in organic semiconductors,
Organic Solar Cells (Sante Fe, NM, **2013**); talk
58. First principles modeling of donor materials for organic solar cells: where theory complements experiment,
APS March Meeting (Baltimore, MD, **2013**); talk
59. First-principles modeling of exciton and charge transport in organic semiconductors: dependence on quantum chemistry method,
ACS Fall Meeting (Philadelphia, PA, **2012**); poster
60. 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
61. 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
62. 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.
63. Charge carrier transport in pi-conjugated systems: stacks versus polymers,
XXVII Southwest Theoretical Chemistry Conference (Lubbock, TX, **2011**); poster
64. What determines the charge state of a soliton in conjugated polymers?,
Int. Conference Optical Probes of Conjugated Polymers (Santa Fe, NM, **2011**); poster
65. An intrinsic formation mechanism for midgap electronic states in semiconductor glasses,
XXV Southwest Theoretical Chemistry Conference (Houston, TX, **2009**); poster
66. Efficient perturbation expansion for disordered systems,
III International Conference Electronics and Applied Physics (Kyiv, Ukraine, **2007**); talk
67. Longtime asymptotics of porous silicon photoluminescence decay,
International Young Scientists Conference on Applied Physics (Kyiv, **2001**); talk
68. Long-time asymptotics of the photoluminescence decay: the role of diffusion and disorder,
NATO/EC Workshop Frontiers of nano-optoelectronic system (Kyiv, **2000**); talk
69. Hopping transport in nanocrystallites structures,
International Conference Advanced Materials (Kyiv, **1999**); poster
70. Hopping transport and photoluminescence in nanocrystallites structures,
Physical Problems in Material Science of Semiconductors (Chernivtsi, Ukraine, **1999**); talk