

# Curriculum Vitae for Andriy Zhugayevych

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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

- 2022-2025 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, electronic coarse-graining, code development.
- **Applied materials science:** organic electronics, energy storage and conversion.
- **Mathematical and theoretical physics and chemistry:** lattice models.

## Most important scientific achievements as principal contributor

- **Organic semiconductors:** contributed to development of first-principles multiscale modeling methods (since **2013**) solving several puzzles on molecular and electronic structure: resolved structure of P3HT polymer (**2018**) and PPV oligomers (**2019**), discovered 3D electronic connectivity in A-D-A materials (**2021**), elucidated charge storage mechanism in metal-organic polymers (**2022**). Methodological achievements include creation of the first benchmark dataset of organic semiconductors (**2023**).
- **Other semiconductors:** discovered small polarons in pnictogens (**2021**); provided a unified picture of pnictides and chalcogenides as ppo-networks (**2010**). Methodological advances include electronic coarse-graining allowing for calculation of electronic structure of nonpolar solids at any DFT level (**2023**); reconstruction of electronic traps distribution from experimental data on phosphorescence kinetics (PhD thesis **2007**).
- **Theoretical physics:** efficient evaluation of lattice Green's functions (**2025**); virial expansion for dynamic correlation function of a lattice gas (**2006**).

See research highlights webpage at <http://zhugayevych.me/research>

## Research experience

2022-2025 Visiting Researcher at Max Planck Institute for Polymer Research:

- **Computational Materials Science of Organic Semiconductors:** Development of methods for first-principles modeling of structural and electronic properties of organic and inorganic semiconductors including electronic-coarse graining and benchmark datasets.

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

- **Computational Materials Science of 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 of Metal-ion Batteries:** Computational screening and in-depth study of electrodes and membranes.

2011-2014 Postdoc at Los Alamos National Laboratory, mentors S. Tretiak and E. Batista:

- **Computational Materials Science of Organic Semiconductors:** 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 of 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:** Various results for the random walk on a disordered lattice are obtained using perturbation theory, mean-field approximation, enumeration techniques etc.

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

- **Statistical Physics:** Dynamic correlation function of a lattice gas derived in cluster expansion.
- **Theoretical Materials Science:** Anomalously slow decay of phosphorescence in porous silicon is explained. Method is developed for retrieving electronic traps distribution from experimental data on phosphorescence kinetics.

1995-1999 PhD student at Institute of Physics, Department of **Theoretical Physics**, mentor B. Lev:

- 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:

- 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:

- Amateur variable star observer. As of 2005, 293 observations submitted 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.html>

## Professional activities

- **Referee** of 27 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, Digit Discov; **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, Coord Chem Rev; **AIP** – J Chem Phys; **APS** – Phys Rev B
- Skoltech **Service:** coordinator of Computational Materials Science Laboratory (2015-2022)
- Skoltech **Service:** coordinator of educational program in Materials Science (2015-2022)
- Skoltech **Service:** coordinator of entry math exam for several programs (2017-2021)
- Skoltech **MSc/PhD Defense** in Materials Science Committee member (2017-2021)
- Kyiv State University **Service:** judging student competitions, recruiting students (2000-2007)
- Institute of Physics (Kyiv) **Service:** establishing Young Scientists Council (2006-2007)
- 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, Python, Fortran – experienced; other computer languages – per-demand use.
- Fluent in Ukrainian and English.

## Grants and Fellowships

- |           |        |                                                                                                                                          |
|-----------|--------|------------------------------------------------------------------------------------------------------------------------------------------|
| 2023-2026 | PI     | CINT user project “Electronic coarse graining of organic semiconductors”, 2022BU0141, 2024AC0125                                         |
| 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                |
| 2015-2021 | PI     | CINT user projects “Modeling of conducting conjugated polymers”, U2015A0016, 2016BC0035, 2018AC0081, 2019BC0120                          |
| 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, [0000-0001-5547-3647](tel:0000-0001-5547-3647)

### Prof. Vassiliy Lubchenko

Chemistry Department  
University of Houston  
Houston, TX 77204, USA  
vas@uh.edu, [0000-0001-6398-261X](tel:0000-0001-6398-261X)

### Prof. Keith Stevenson

1) Center for Energy Science and Technology  
Skoltech as MIT Initiative, Moscow 2013-2022  
2) Watts kWh, LLC, Austin, TX, USA  
kjsaustin@msn.com, [0000-0002-1082-2871](tel:0000-0002-1082-2871)

### Dr. Andriy Kadamashchuk

1) Institute of Physics, Kyiv, Ukraine  
2) University of Bayreuth, Germany  
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[0000-0001-8459-7825](tel:0000-0001-8459-7825)

## List of Publications

[Google Scholar profile](#): 1200 citations, h-index 22, h5-index 18, i10-index 30

[Scopus/WoS](#) h-index is 19; SciVal FWCI 2015-2021 is 1.51 (1.69 for Materials Science)

See also electronic Handbooks and Lecture Notes at <http://zhugayevych.me/handbooks.html>

Other open scientific content is listed in "Scientific pages" section at <http://zhugayevych.me>

### Peer-reviewed publications

1. Fluorinated Polythiophenes with Ester Side Chains for Boosting the V and Efficiency in Non-Fullerene Polymer Solar Cells,  
L Su, Y Zhou, Y Chen, G Chen, K Tseng, N Tukachev, **A Zhugayevych**, S Tretiak, L Wang,  
*Polymer* 326, 128336 (2025) 10.1016/j.polymer.2025.128336 IF2023=4.1, Q1
2. Efficient evaluation of lattice Green's functions,  
**A Zhugayevych**,  
*J Phys A* 58, 025209 (2024) 10.1088/1751-8121/ada0fb IF2023=2.0, Q1
3. Benchmark Data Set of Crystalline Organic Semiconductors,  
**A Zhugayevych**, W Sun, T van der Heide, C Lien-Medrano, T Frauenheim, S Tretiak,  
*J Chem Theory Comput* 19, 8481 (2023) 10.1021/acs.jctc.3c00861 IF2022=5.5, Q1
4. Electronic coarse-graining of long conjugated molecules: Case study of non-fullerene acceptors,  
**A Zhugayevych**, K Lin, D Andrienko,  
*J Chem Phys* 159, 024107 (2023) 10.1063/5.0155488 IF2021=4.3, Q1
5. Variational polaron equations applied to the anisotropic Frohlich model,  
V Vasilchenko, **A Zhugayevych**, X Gonze,  
*Phys Rev B* 105, 214301 (2022) 10.1103/PhysRevB.105.214301 IF2021=3.9, Q1,NI
6. Charge storage mechanisms of a pi-d conjugated polymer for advanced alkali-ion battery anodes,  
R Kapaev, **A Zhugayevych**, S Ryazantsev, D Aksyonov, D Novichkov, P Matveev, K Stevenson,  
*Chem Sci* 13, 8161 (2022) 10.1039/D2SC03127B IF2021=10, Q1,NI
7. 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
8. 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.jpcllett.1c00929 IF2019=6.7, Q1,NI
9. Hydroxyl Defects in LiFePO<sub>4</sub> 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

10. 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
11. 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
12. Reversible electrochemical potassium deintercalation from >4 V positive electrode material K<sub>6</sub>(VO)<sub>2</sub>(V<sub>2</sub>O<sub>3</sub>)<sub>2</sub>(PO<sub>4</sub>)<sub>4</sub>(P<sub>2</sub>O<sub>7</sub>),  
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
13. 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
14. 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
15. Correlating structure and transport properties in pristine and environmentally-aged superionic conductors based on Li<sub>1.3</sub>Al<sub>0.3</sub>Ti<sub>1.7</sub>(PO<sub>4</sub>)<sub>3</sub> 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
16. 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
17. 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.jpcllett.9b01572 IF2017=8.7, Q1,NI
18. 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.jpcllett.9b01200 IF2017=8.7, Q1,NI
19. 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

20. Reversible facile Rb<sup>+</sup> and K<sup>+</sup> ions de/insertion in a KTiOPO<sub>4</sub>-type RbVPO<sub>4</sub>F 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
21. 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
22. 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
23. Single crystal microwires of *p*-DTS(FBTTh<sub>2</sub>)<sub>2</sub> 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
24. 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
25. Crystal structure and Li-ion transport in Li<sub>2</sub>CoPO<sub>4</sub>F 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
26. 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
27. 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
28. 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
29. 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

30. 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
31. 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
32. 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
33. 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
34. 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
35. 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
36. Electronic structure and the glass transition in pnictide and chalcogenide semiconductor alloys. I. The formation of the  $pp\sigma$ -network,  
**A Zhugayevych**, V Lubchenko,  
*J Chem Phys* 133, 234503 (**2010**); arXiv: 1006.0771 10.1063/1.3511707 IF2010=2.9, Q1
37. 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
38. Dynamic correlations in an ordered  $c(2\times 2)$  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
39. Charge pump effect and mechanisms of charge carriers localization in oxidized nano-Si,  
I V Blonsky, V Kadan, A Kadashchuk, A Vakhnin, **A Zhugayevych**,  
*Int J Nanotechnology* 3, 65 (**2006**) 10.1504/IJNT.2006.008721 Q2
40. Approximate calculation of operator semigroups by perturbation of generators,  
A Yurachivsky, A Zhugayevych, *Reports Nat Acad Sci Ukraine* 11, 27 (**2003**)



41. 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**)
42. 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**)
43. 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
44. 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

45. 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](https://doi.org/10.1007/978-3-030-31866-6_2)
46. Mathematical physics in problems and solutions,  
A. Yurachivsky, **A. Zhugayevych**, (Kyiv Univ., **2005**), 158 pages, in ukrainian
47. 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. Zherebetsky, A. Khomenko, I. Sporysh, in *Frontiers of Multifunctional Integrated Nanosystems*, ed. E. Buzaneva, P. Scharff, p. 251 (Kluwer, **2004**)

### Invited presentations

48. Electronic coarse-graining of semiconductors: methodology and applications,  
*TUM Seminar on Theory and Computation of Materials and Molecules* (Munich, **2024**)
49. Nonadiabatic dynamics at large scales from perspective of applications to organic semiconductors,  
*Virtual International Seminar on Theoretical Advancements* 44 (online, **2022**)
50. Electronic coarse-graining of organic semiconductors: methods and applications,  
*Bremen Center for Computational Materials Science Seminar* (Bremen, **2022**)
51. Computational studies of organic semiconductors,  
*1st International School on Hybrid, Organic and Perovskite Photovoltaics* (Moscow, **2019**)
52. Modeling of electronic properties of organic semiconductors,  
*Inaugural Symposium for Computational Materials Program of Excellence* (Moscow, **2019**)
53. Modeling of charge transport in materials for energy and optoelectronics,  
*LANL Center for Nonlinear Studies Colloquium* (Los Alamos, NM, **2017**)

54. Modeling of conjugated polymers: non-oligomer approach,  
*Telluride workshop Nonequilibrium Phenomena, Nonadiabatic Dynamics and Spectroscopy* (Telluride, CO, **2017**)
55. First-principle modeling of energy and charge transport in organic semiconductors,  
*3rd International Fall School on Organic Electronics* (Moscow, **2016**)
56. First-principle effective Hamiltonian modeling of charge and energy transfer in molecular systems: Picosecond-scale phenomena,  
*Mesilla Chemistry Workshop Electrochemical Processes* (Mesilla, NM, **2016**)
57. First principle modeling of materials for organic electronics,  
*Institute of Physics, Department of Theoretical Physics Colloquium* (Kyiv, **2014**)
58. Multiscale modeling of nanomaterials with application to organic solar cells,  
*Massachusetts Institute of Technology, MIT Skoltech Initiative* (Boston, MA, **2014**)
59. Ultrafast exciton dissociation in small-molecule bulk-heterojunction solar cells,  
*Telluride conference on Advances in Photoreactions* (Telluride, CO, **2013**)
60. Midgap electronic states in amorphous pnictide and chalcogenide semiconductors,  
*LANL Center for Integrated Nanotechnologies Colloquium* (Los Alamos, NM, **2011**)

### Contributed presentations (since 2007)

61. Charge storage mechanism in metal-organic polymers for alkali-ion battery electrodes,  
*UHMob International Conference - Organic Semiconductors* (Mainz, **2022**); talk
62. Comparison of non-fullerene acceptors: How geometry influences electronic transport,  
*2nd Int. School on Hybrid, Organic and Perovskite Photovoltaics* (Moscow, **2020**); talk
63. Polymorphism and charge transport in organic semiconductors,  
*4th International Fall School on Organic Electronics* (Moscow, **2018**); talk
64. Challenges in Computational Design of Organic Semiconductors,  
*14th International Conference on Organic Electronics* (Bordeaux, **2018**); poster
65. Towards rational design of organic solar cells: How to control the structure of bulk material,  
*Atomistic Simulation of Functional Materials* (Moscow, **2014**); talk
66. Exciton transport in a crystal of soft molecules beyond small polaron hopping,  
*Excited State Processes* (Santa Fe, NM, **2014**); poster
67. Multiscale modeling of exciton and charge carrier transport in organic semiconductors,  
*Organic Solar Cells* (Sante Fe, NM, **2013**); talk
68. First principles modeling of donor materials for organic solar cells: where theory complements experiment,  
*APS March Meeting* (Baltimore, MD, **2013**); talk
69. First-principles modeling of exciton and charge transport in organic semiconductors: dependence on quantum chemistry method,  
*ACS Fall Meeting* (Philadelphia, PA, **2012**); poster
70. 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

71. First-principles study of energy/charge transport in molecular donors for organic solar cells, *LANL Postdoc Research Day* (Los Alamos, NM, **2012**); poster
72. Understanding the high device efficiency of a class of solution-processed small-molecule solar cells, *APS March Meeting* (Boston, MA, **2012**); talk
73. Charge carrier transport in pi-conjugated systems: stacks versus polymers, *XXVII Southwest Theoretical Chemistry Conference* (Lubbock, TX, **2011**); poster
74. What determines the charge state of a soliton in conjugated polymers? *Int. Conference Optical Probes of Conjugated Polymers* (Santa Fe, NM, **2011**); poster
75. An intrinsic formation mechanism for midgap electronic states in semiconductor glasses, *XXV Southwest Theoretical Chemistry Conference* (Houston, TX, **2009**); poster
76. Efficient perturbation expansion for disordered systems, *III International Conference Electronics and Applied Physics* (Kyiv, Ukraine, **2007**); talk