

CURRICULUM VITAE (CV)

1. Personal information

Name: **Janis Timosenko** (*Janis Timoshenko, Jānis Timošenko*)
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2. Education

Higher education:

- 2010 – 2015 University of Latvia, Physics, Astronomy and Mechanics Doctoral Study Program (*Latvijas Universitāte, Fizikas, astronomijas un mehānikas doktora studiju programma*). Graduated on 04/03/2015.
Doctoral degree in condensed matter physics (*Fizikas doktora zinātniskais grāds cietvielu fizikā*) earned.
- 2008 – 2010 University of Latvia, Physics Master Study Program (*Latvijas Universitāte, Fizikas maģistra studiju programma*). Graduated on 07/04/2010.
Master degree in Physics (*Dabaszinātņu maģistra grāds fizikā*) earned.
- 2005 – 2008 University of Latvia, Physics Bachelor Study Program (*Latvijas Universitāte, Fizikas bakalaura studiju programma*). Graduated on 07/04/2008.
Bachelor degree in Physics (*Dabaszinātņu bakalaura grāds fizikā*) earned.

Languages:

- 1) Latvian – fluent in written and spoken
- 2) Russian – mother tongue
- 3) English – fluent in written and spoken
- 4) German – intermediate level of written and spoken language
- 5) Italian – beginner level

Computer skills

- 1) Operating systems: *MS Windows (XP, Vista, 7, 8, 10, 11), MS DOS, Linux*
- 2) Office applications: *MS Office, OpenOffice, Latex, Inkscape, Origin*
- 3) CAD software: *some experience with SolidWorks and TurboCad*
- 4) Molecular dynamics software: *GULP, also some experience with LAMMPS*
- 5) EXAFS data analysis software: *FEFF, Athena, FEFFIT, EDA, Larch, FDMNES*
- 6) Programming and scripting languages: *C/C++, Wolfram Mathematica, GNUplot, also some experience with Pascal, Python, Labview, Matlab, R, HTML*

3. Employment history

- 2018 – present Fritz-Haber Institute of Max Planck Society, Department of Interface science, group leader
- 2016 – 2018 Stony Brook University, Department of Materials Science and Chemical Engineering, postdoctoral scholar
- 2015 – 2016 Yeshiva University, Physics Department, postdoctoral scholar
- 2013 – 2015 University of Latvia, Institute of Solid State Physics, researcher
- 2012 – 2015 University of Latvia, Faculty of Physics and Mathematics, researcher
- 2009 – 2012 University of Latvia, Faculty of Computing, science assistant
- 2006 – 2009 University of Latvia, Faculty of Physics and Mathematics, programming engineer

4. Research expertise and interests

a) Areas of expertise: material science, nanocatalysis, X-ray absorption spectroscopy, in-situ XAS studies, advanced XAS data analysis, machine learning methods, atomistic simulations techniques (molecular dynamics, reverse Monte Carlo methods), global optimization techniques (simulated annealing, evolutionary algorithms), linear algebra methods (principal component analysis, multivariate curve resolution/blind source separation method), theoretical physics (mesoscopic charge transport, quantum computing, statistical physics), some experience with computational fluid dynamics.

b) Current research interests: experimental investigations of materials with time-resolved XAS method to link the structural and dynamical information from XAS with materials properties and function. I am particularly interested in the development and application of advanced data analysis approaches to fully benefit from the information, encoded in X-ray absorption spectra, and also in combination of experimental measurements with the results of theoretical modelling.

c) Participation in experiments at synchrotron radiation facilities; experience with XAS:

I have participated in XAS experiments at BESSY, DORIS, PETRA III and ANKA (Germany), SLS (Switzerland) ELETTRA (Italy), SOLEIL, ESRF (France), ALBA (Spain), SSRL, NSLS-II APS (USA) synchrotron radiation facilities, including measurements in fluorescence, transmission modes and grazing incidence modes, temperature-dependent, pressure-dependent XAS measurements, operando investigations of catalytic processes, RIXS measurements (APS, ESRF), measurements in QXAFS mode (NSLS-II, SOLEIL, SLS and DESY), X-ray Raman scattering experiments (ESRF) and measurements with optically dispersed setup (SOLEIL). Also, I have some experience with FTIR measurements at SOLEIL synchrotron and synchrotron-based XRD (NSLS II and DESY). Currently I am also leading the team responsible for designing the new Max Planck Society-funded beamline at PETRA III/IV, devoted to operando studies of catalysts using XAS, XRD, SAXS and XES methods. Furthermore, me and my group at FHI are currently working on adapting the new lab-based XAS spectrometer for operando investigations of catalysts. I have co-authored more than 100 papers on XAS studies, including those on advanced approaches for XAS data analysis.

d) Participation in major research projects:

Extension of CatLab research platform (German Federal Ministry of Education and Research (BMBF) and Max-Planck Society funding): co-proposer with Prof. Beatriz Roldan Cuenya for beamline front-end station for PETRA synchrotron, 2021 - *present*

U.S. National Science Foundation Project *Toolkit to Characterize and Design Bi-functional Nanoparticle Catalysts* under DMREF program (collaboration project, involving Yeshiva University/Stony Brook University, University of Texas in Austin, University of Pittsburgh), 2015 – 2018.

EUROFUSION projects *When and how ODS particles are formed? - X-ray Absorption Spectroscopy and ab initio modelling of ODS steels* and *ODS steel with high creep strength* (collaboration project of University of Latvia with Karlsruhe Institute of Technology (Germany) and CIEMAT (Spain)), 2014-2015.

EURATOM projects *Production and characterization of laboratory-scale batches of nano-structured ODSFD* and *Experimental validation of models* (collaboration project of University of Latvia with Karlsruhe Institute of Technology (Germany) and University of Helsinki (Finland), 2013 – 2015.

e) participation in summer schools and workshops

- 1) *Summer School on Atomistic Simulation Techniques* (04.07.2010. – 25.07.2010, Trieste, Italy);
- 2) *Ultrafast X-Ray Science with X-Ray Free-Electron Lasers* (29.03.2011. – 02.04.2011, DESY Hamburg, Germany);
- 3) *32nd Berlin School on neutron scattering* (07.03.2012. – 16.03.2012, HZB, Berlin, Germany).
- 4) *HERCULES-2013 (Higher European Research Course for Users of Large Experimental Systems)* (24.02.2013 - 28.03.2013, ESRF, Grenoble, France).

5) *HERCULES Specialized Course on Dynamical properties investigated by neutrons and synchrotron X-rays* (15.09.2014 - 19.09.2014, ESRF, Grenoble, France).

5. Teaching experience

a) Teaching positions

- 2021 – present Teaching position in Statistical Physics/ Faculty for Physics and Mathematics, University of Latvia, Latvia
- 2013 – 2015 Teaching assistant – Quantum Theory / Faculty for Physics and Mathematics, University of Latvia, Latvia

b) Supervision of students and postdoctoral fellows

- 2020 – *present* Direct supervision of 3 Postdocs (Dr. U. Hejral, Dr. A. Martini, Dr. J. Jang) and 1 PhD student (M. Rüscher). Co-supervision of 7 PhD students (C. Rettenmaier, A. Herzog, F.T. Haase, D. Kordus, M. Lopez-Luna, E. Liberra, L. Proano) at the Interface Science Department at Fritz Haber Institute of Max Planck Society, Germany
- 2013 – 2015 Supervision of 1 undergraduate student (I. Jonane-Pudza) at the Institute of Solid State Physics at University of Latvia, Latvia

c) Other teaching activities

- 2006 – *present* Co-organizer of Latvian Physics Olympiads for high school students, Latvia

6. Institutional responsibilities

- 2008 – 2014 Member of Council of Physics Study Program of Physics department, University of Latvia;

7. Organization of scientific meetings

- 2021 Co-organizer of European Nanoanalysis Symposium at European Materials Research Society Fall Meeting 2021
- 2016–2023 Co-organizer of “XAFS Short Course” workshops, Brookhaven National Lab, USA

8. Awards and recognition

2022 - Farrel Lytle Prize (Young Scientists Award for Theory and Instrumentation) of the International X-Ray Absorption Society (IXAS)

2016 - Presidential Award of Latvian Academy of Sciences for the work on "Pressure-induced insulator to metal phase transition in tin tungstate", authors - A. Kuzmin, A. Anspoks, A. Kalinko, **J. Timoshenko** and R. Kalendarev.

2015 – Award of Latvian Academy of Sciences for the young scientists (Ludvigs and Māris Jansons prize for the best work in physics).

2014 – Award of Latvian Academy of Sciences for a significant achievement in theoretical science (for the new method for investigations of structural and thermal disorder in crystalline and nanocrystalline materials using X-ray absorption spectroscopy and evolutionary algorithm approach, authors – **J. Timoshenko**, A. Anspoks, A. Kalinko, A. Kuzmin, J. Purans).

2012 – Award of Latvian Academy of Sciences for a significant achievement in theoretical science (for

the new approach for quantum algorithms design and new application of quantum interference in nanoelectronics, authors - A. Ambainis, V. Kashcheyevs, A. Belovs, **J. Timoshenko**).

9. Membership of scientific societies

2018 – present Member of International X-ray Absorption Society

2017 – present Member of American Chemical Society

10. Reviewing activities

2006 – *present* Scientific paper reviewing, including manuscripts submitted to ACS Catalysis, ACS Applied energy materials, ACS Energy Letters, Journal of Physical Chemistry Letters, Journal of Physical Chemistry, Chemical Reviews, Angewandte Chemie, Crystals, Chemistry of Materials, Physica Status Solidi B, Physical Chemistry Chemical Physics, Nature Communications, Nature Catalysis, ChemCatChem, Chem-Catalysis, Catalysts, Minerals, Computational Materials Science, Molecular Simulation, Patterns, Advanced Materials, Joule

Evaluation of scientific grant application proposals for DFG (2022), Israel Science Foundation (2022), Vietnam National Foundation for Science and Technology (2021)

11. Most significant publications

Total number of publications (published or accepted for publication): 111, h-index: 37, ORCID 0000-0003-2963-3912

- 1) **J. Timoshenko**, F. T. Haase, S. Saddeler, M. Rüscher, H. S. Jeon, A. Herzog, U. Hejral, A. Bergmann, S. Schulz, B. Roldan Cuenya, *Deciphering the structural and chemical transformations of oxide catalysts during oxygen evolution reaction using quick X-ray absorption spectroscopy and machine learning*, J. Am. Chem. Soc. 145, 4065 (2023) (**journal impact factor (IF) 16.4**)
- 2) **J. Timoshenko**, A. Bergmann, C. Rettenmaier, A. Herzog, R. M. Arán-Ais, H. S. Jeon, F. T. Haase, U. Hejral, P. Grosse, S. Köhl, E M. Davis, J. Tian, O. Magnussen, B. Roldan Cuenya, *Steering the structure and selectivity of CO₂ electroreduction catalysts by potential pulses*, Nature Catal. 5, 259 (2022) (**journal IF 40.7**)
- 3) **J. Timoshenko**, B. Roldan Cuenya, *In situ/operando electrocatalyst characterization by X-ray absorption spectroscopy*, Chem. Rev. 121, 882 (2021) (**review paper; journal IF 54.3**)
- 4) **J. Timoshenko**, A. Anspoks, A. Cintins, A. Kuzmin, J. Purans, A. I. Frenkel, *Neural Network Approach for Characterizing Structural Transformations by X-Ray Absorption Fine Structure Spectroscopy*, Phys. Rev. Lett. 120, 225502 (2018) (**journal IF 9.2**)
- 5) **J. Timoshenko**, D. Lu, Y. Lin, A.I. Frenkel, *Supervised machine learning-based determination of three-dimensional structure of metallic nanoparticles*, J. Phys. Chem. Lett. 8, 5091 (2017) (**highlighted in the virtual issue of The Journal of Physical Chemistry on Machine Learning; journal IF 6.7**)

12. Patents

US Patent 11193884 *System and method for structural characterization of materials by supervised machine learning-based analysis of their spectra* (A.I. Frenkel, **J. Timoshenko**), 2021

13. Most significant conference presentations

Invited talks at major international conferences:

- 1) *Understanding the Dynamic Structure of Working Electrocatalysts Using Operando QXAFS See the abs*, E-MRS Fall Meeting 2023 (Warsaw, Poland)
- 2) *Tracking the evolution of copper clusters, nanoparticles and nanocubes by time-resolved X-ray absorption spectroscopy and machine learning*, Clusters Meeting 2023 (Prague, Czech Republic)
- 2) *Understanding the structure-properties relationship in nanocatalysts for CO₂ electroreduction using time-resolved XAS and advanced data analysis*, 4 Joint AIC - SILS Conference (Trieste, Italy, 2022)
- 3) *Tracking the structure and composition of copper-based catalysts for CO₂ electroreduction using operando XAS*, ACS Spring Meeting 2021 (online)
- 4) *Probing disorder in nanoparticles using in-situ X-ray absorption spectroscopy and machine learning*, E-MRS Spring Meeting 2021 (online)
- 5) *In situ/operando electrocatalyst characterization by X-ray absorption spectroscopy*, Chemical Reviews Virtual Lecture Series (2021, online)
- 6) *Probing atomic-scale structure and dynamics in metallic nanocatalysts by x-ray absorption spectroscopy and theoretical simulations*, ACS 254th National Meeting, (2017, Washington, USA)

Invited talks at workshops and summer schools:

- 1) *Tracking and steering the dynamic structures of single atom catalysts for electrocatalytic CO₂ reduction reaction using operando XAS*, DESY User meeting (Hamburg, 2024)
- 2) *Challenges and opportunities for machine learning in XAS data interpretation*, ALBA II Symposium, Universidad Autónoma de Madrid (Madrid, Spain, 2024)
- 3) *Machine Learning Methods*, EXAFS 50 Symposium, Brookhaven National Lab (Upton, USA, 2023)
- 4) *Obtaining 3D structure from EXAFS spectra*, XAFS Short Course, Brookhaven National Lab (Upton, USA, 2023)
- 5) *Improving the interpretation of XAS data using artificial neural networks*, Q2XAFS 2023 (International Workshop on Improving Data Quality and Quantity in XAFS Spectroscopy), Australian Synchrotron (Melbourne, 2023)
- 6) *In situ/Operando X-ray Absorption Spectroscopy*, HZB Photon School (2019, 2020, 2021, 2022, 2023 Berlin & online)
- 7) *Tracking the evolution of heterogeneous structures in working catalysts using machine learning*, DESY User meeting (Hamburg, 2023)
- 8) *Multiple scattering EXAFS analysis and measuring bond length disorder by EXAFS*, XAFS Short Course 2022 (on-line)
- 9) *Tracking the compositional and chemical changes in working electrocatalysts using unsupervised and supervised machine learning*, 2nd workshop on Correlative Materials Characterization, (Dresden, 2022),
- 10) *Basic and advanced analysis of extended X-ray absorption fine structure*, HZB Photon School (2021, 2022 on-line)
- 11) *Probing kinetics of catalyst transformations using synchrotron based operando techniques and machine learning*, invited plenary lecture at 6th International School-Conference on Catalysis for Young Scientists “Catalyst Design: From Molecular to Industrial Level” (2021, on-line)
- 12) *Machine learning algorithms for the analysis of spectroscopy data*, Correlative Materials

Characterization, DGM European Advanced Training Course (2021, on-line)

- 13) *Reverse Monte Carlo modelling and neural networks in EXAFS analysis*, Advanced XAS Data Analysis and Modeling Virtual Workshop, Canadian Light Source, (2020, on-line)
- 14) *Extracting nanoscale details from X-ray absorption data by supervised machine learning*, NSLS-II and CFN Users' Meeting (Brookhaven National Lab, USA, 2018)