Rafał Topolnicki

Dioscuri Centre in Topological Data Analysis
Mathematical Institute
Polish Academy of Sciences

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Position

Visiting Assistant Professor (Adiunkt) **since Oct 2021**

Mathematical Institute of the Polish Academy of Sciences

Assistant Professor (Adiunkt) **since Oct 2017 (on leave)**

University of Wrocław, Faculty of Physics and Astronomy

Education

Ph.D. in Mathematics [Mathematical Statistics] **Oct 2020**

Wrocław University of Science and Technology
thesis: *Semiparametric estimation of the ROC curve*

Ph.D. in Physics [Solid State Physics] (with distinction) **Dec 2017**

University of Wrocław
thesis: *Theoretical study of the adsorption and coadsorption of Sn and Pb on Ru(0001)*

M.Sc. in Mathematics (graduated with distinction) **Jul 2014**

Wrocław University of Science and Technology
specialization: Mathematical Statistics
thesis: *Semiparametric estimation of ROC curve*

M.Sc. Physics (graduated with distinction) **Jul 2012**

University of Wrocław, Faculty of Physics and Astronomy
specialization: physics of new materials
thesis: *Structural and electronic properties of the Ni/W(111) and Co/W(111) adsorption systems*

B.Sc in Physics, B.Sc. in Mathematics **2010,2012**

Postdocs

Dioscuri Centre in Topological Data Analysis, dr hab. Paweł Dłotko group **since 10.2021**

Mathematical Institute of the Polish Academy of Sciences
topic: applications of topological data analysis to statistics, material science and machine learning

Lehrstuhl für Theoretische Chemie, prof. Domnik Marx group **07.2019-06.2020**

Ruhr-Universität Bochum
topic: appying neural network potential for molecular dynamics simulations to study temperature dependant correlations in large amplitude motion of fluxional molecules under quantum delocalization effects

International Studies

University of Tromsø, Norway **Aug-Dec 2011**

Erasmus exchange programme. Studies focused on Mathematical Statistics and Quantum Chemistry

Internships

1. Max Planck Insitute for Mathematics, Lepizig, **Jul 2022**
2. Institute of Physics, Czech Academy of Sciences, Prague **Dec 2013**
3. Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw **Sep-Dec 2012**

4. Joint Institute of Nuclear Research, Dubna **Jul 2011**
5. Institute for Chemical Processing of Coal, Zabrze **Feb 2011**
6. Institute of Low Temperature and Structural Research, Polish Academy of Sciences, Wrocław **Jul-Sep 2010**

Publications in advanced preparation

1. *Generalization of CNN predictions of pore-scale flow through porous media*
2. *Robust Importance Sampling for Rare Events via Cross-Entropy with Constrained Gaussian Mixtures*
3. *Using direction-aware topological data analysis to improve the prediction of Young's modulus in porous materials*
4. *Reducing Estimation Uncertainty Using Normalizing Flows and Stratification*

Publications under review

1. *Transferable 3D Convolutional Neural Networks for Elastic Constants Prediction in Nanoporous Metals*, in: Materials and Design
2. *Estimation of conditional inequality curves and measures via estimating the conditional quantile function*, in: Statistics and Computing

Publications

24. *Violation of Matthias rule: Elemental composition as the key determinant of critical temperature in bcc high-entropy superconductors*
Physical Review B **112**, 014513 (2025)
23. *Interpretable machine learning for atomic scale magnetic anisotropy in quantum materials*
npj Computational Materials **11**, 138 (2025)
22. *New type of Ti-rich HEA superconductors with high upper critical field*
Acta Materialia **285**, 120666 (2025)
21. *Superconductivity in a New High-Entropy Alloy (NbTi)0.67 (MoHfV)0.33*
Metallurgical and Materials Transactions A **55**, 3789-3898 (2024)
20. *Topology-driven goodness-of-fit tests in arbitrary dimensions*
Statistics and Computing **34**, 34 (2024)
19. *Superconductivity in high-entropy alloy system containing Th*
Scientific Reports **13**, 16317 (2023)
18. *Enhanced Superconducting Critical Parameters in a New High-Entropy Alloy Nb0.34Ti0.33Zr0.14Ta0.11Hf0.08*
Materials **16(17)**, 5814 (2023)
17. *Deciphering the Impact of Helium Tagging on Flexible Molecules: Probing Microsolvation Effects of Protonated Acetylene by Quantum Configurational Entropy*
Journal of Physical Chemistry A **127**, 11 (2023)
16. *Superconductivity in the high-entropy alloy* $(NbTa)_{0.67}(MoHfW)_{0.33}$
Physical Review B **106**, 184512 (2022)
15. *Minimum distance estimation of the Lehmann ROC curve*
Statistics **55**, 618 (2021)
14. *Combining multiscale MD simulations and machine learning methods to study electronic transport in molecular junctions at finite temperatures*
Chemical Physics Letters **125,36**, 19961 (2021)
13. *Temperature driven interchange of the effective size of proton with deuterium*
Chemical Physics Letters **778**, 138775 (2021)
12. *Deciphering High-Order Structural Correlations within Fluxional Molecules from Classical and Quantum Configurational Entropy*
Journal of Chemical Theory and Computation **16,11**, 6785-6794 (2020)
11. *Estimation of the ROC curve from the Lehmann family*
Computational Statistics & Data Analysis **142**, 106820 (2020)

10. *Characterization of (In,Pb)/Si(111): Tuning normal and lateral atom distributions in mixed metal systems*
Journal of Alloys and Compounds **819**, 153030 (2020)
9. *Minimum distance estimation of the binormal ROC curve*
Statistical Papers **60**, 2161-2183 (2019)
8. *Early stages of growth of Pb, Sn and Ge on Ru(0001): A comparative density functional theory study*
Thin Solid Films **665**, 123-130 (2018)
7. *Estimation of the Ratio of the Geometric Process*
Applicationes Mathematicae **44**, 105-121 (2017)
6. *Tuning the conductance of benzene-based single-molecule junctions*
Org. Electron. **34**, 254-261 (2016)
5. *On the formation of two-dimensional alloys of Sn and Pb co-adsorbed on Ru(0001)*
J. Alloys Compd. **672**, 317–323 (2016)
4. *Structural and electronic properties of submonolayer-thick Sn films on Ru(0001)*
Appl. Surf. Sci. **329**, 376–383 (2015)
3. *Structural properties of ultrathin Pb layers on Ru(0 0 0 1) revealed by LEED, AES and DFT*
Appl. Surf. Sci. **311**, 426–434 (2014)
2. *Electronic properties of experimentally observed Pb/Ru(0 0 0 1) adsorbate structures: A DFT study*
Appl. Surf. Sci. **304**, 115-121 (2014)
1. *Phase diagram for a zero-temperature Glauber dynamics under partially synchronous updates*
Phys. Rev. E **86**, 051113 (2012)

Grants (as PI only)

1. NAWA Bekker Programme PPN/BEK/2018/1/00319: *Introducing neural networks to quantum-mechanical study of chemical reactions in superfluid helium environment*
2. NCN Preludium project 2016/23/N/ST3/00008: *Electronic transport properties of molecular junctions: A novel approach to include temperature effects*
3. various grants for supercomputer time

Oral Presentations At Conferences

10. GAMM2025 - Annual Meeting of the International Association of Applied Math. and Mechanics Poznań 10.04.2025
Prediction of elastic modulus for metallic porous materials using 3D convolution neural networks
9. MSML 2025 - 3rd International Seminar on Modelling, Simulation and Machine Learning for the Rapid Development of Porous Materials Keele 25.03.2025
Prediction of Elastic Properties and Fluid Flow in Porous Media Using Neural Networks
8. 2024 International Workshop on Surface Physics Niemcza 24.09.2024
Magnetic anisotropy energy in graphene-supported atomic-scale magnets: machine learning combined with the DFT calculations
7. Konferencja Naukowej Sekcji Klasyfikacji i Analizy Danych PTS Warszawa 07.09.2022
Zastosowanie metod topologicznych do konstrukcji wielowymiarowych testów zgodności
6. Applied Topology Będlewo, 08.07.2022
TopoTests. One- and two-sample statistical tests motivated by topology
5. 32nd European Conference on Surface Science Grenoble, 30.08.2016
van der Waals density-functional study for low-index metallic surfaces
4. 31st European Conference on Surface Science Barcelona, 02.09.2015
Single and binary films of immiscible Sn and Pb metals on Ru(0001)
3. 7th International Workshop on Surface Physics Trzebnica, 25.06.2015
On the formation of two-dimensional alloys of Sn and Pb co-adsorbed on Ru(0001)
2. 12th Workshop on Stochastic Models, Statistics and Their Applications Wrocław, 17.02.2015
Estimation of the ratio of the geometric process
1. 7+ poster presentations