



Dioscuri Centre for TDA
Institute of Mathematics of the
Polish Academy of Sciences

Rafał Topolnicki

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POSITION

- Post-doc at Dioscuri Centre for TDA** since Oct 2021
Institute of Mathematics of the Polish Academy of Sciences
- Software Developer, ML engineer** 2018-2019,2020-
MicroscopeIT (Tooploox)
- Assistant Professor (Adiunkt)** since Oct 2017 (currently 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

- Lehrstuhl für Theoretische Chemie, prof. Dominik Marx group** 07.2019-06.2020
Ruhr-Universität Bochum
topic: applying 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

- ▶ Institute of Physics, Czech Academy of Sciences, Prague (Czech Republic) Dec 2013
- ▶ Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw Sep-Dec 2012
- ▶ Joint Institute of Nuclear Research, Dubna (Russia) Jul 2011
- ▶ Institute for Chemical Processing of Coal, Zabrze Feb 2011

SKILLS

Programming Languages

python

R

C++

bash

Foreign Languages: English (C1)

AWARDS

Software

various quantum chemical

simulation packages

Keras/Tensorflow

git

- ▶ Scholarship granted by Polish Minister of Science and Higher Education (twice)
- ▶ Annually awarded a scholarship for best PhD students
- ▶ Finalist for the French Vacuum Society *Michel Cantarel* student grants

PUBLICATIONS

- ▶ *Combining multiscale MD simulations and machine learning methods to study electronic transport in molecular junctions at finite temperatures*
J. Phys. Chem. C **125,36**, 19961-19968 (2021)
- ▶ *Temperature driven interchange of the effective size of proton with deuterium*
Chemical Physics Letters **778**, 138755 (2021)
- ▶ *Minimum distance estimation of the Lehmann ROC curve*
Statistics **55**, 618-634 (2021)
- ▶ *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)
- ▶ *Estimation of the ROC curve from the Lehmann family*
Computational Statistics & Data Analysis **142**, 106820 (2020)
- ▶ *Characterization of (In,Pb)/Si(111): Tuning normal and lateral atom distributions in mixed metal systems*
Journal of Alloys and Compounds **819**, 153030 (2020)
- ▶ *Minimum distance estimation of the binormal ROC curve*
Statistical Papers **60**, 2161-2183 (2019)
- ▶ *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)
- ▶ *Estimation of the Ratio of the Geometric Process*
Applicationes Mathematicae **44**, 105-121 (2017)
- ▶ *Tuning the conductance of benzene-based single-molecule junctions*
Org. Electron. **34**, 254-261 (2016)
- ▶ *On the formation of two-dimensional alloys of Sn and Pb co-adsorbed on Ru(0001)*
J. Alloys Compd. **672**, 317-323 (2016)
- ▶ *Structural and electronic properties of submonolayer-thick Sn films on Ru(0001)*
Appl. Surf. Sci. **329**, 376-383 (2015)
- ▶ *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)
- ▶ *Electronic properties of experimentally observed Pb/Ru(0 0 0 1) adsorbate structures: A DFT study*
Appl. Surf. Sci. **304**, 115-121 (2014)
- ▶ *Phase diagram for a zero-temperature Glauber dynamics under partially synchronous updates*
Phys. Rev. E **86**, 051113 (2012)

GRANTS (AS PI ONLY)

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

ORAL PRESENTATIONS AT INTERNATIONAL CONFERENCES

- ▶ 32nd European Conference on Surface Science
van der Waals density-functional study for low-index metallic surfaces Grenoble, 30.08.2016
- ▶ 31st European Conference on Surface Science
Single and binary films of immiscible Sn and Pb metals on Ru(0001) Barcelona, 02.09.2015
- ▶ 7th International Workshop on Surface Physics
On the formation of two-dimensional alloys of Sn and Pb co-adsorbed on Ru(0001) Trzebnica, 25.06.2015
- ▶ 12th Workshop on Stochastic Models, Statistics and Their Applications
Estimation of the ratio of the geometric process Wrocław, 17.02.2015
- ▶ 5+ poster presentations

COURSES, WORKSHOPS ETC.

- ▶ *FAU Physics Academy 2016: Oxides and their Surfaces* Mar 2016
Friedrich-Alexander-University of Erlangen-Nuremberg
- ▶ *3rd workshop on surface structures Electron Diffraction for Quantitative Surface Structure Determination* Jul 2015
University of Łódź
- ▶ *CECAM workshop: juDFT: Hands-on DFT codes from Jülich* Sep 2014
Forschungszentrum Jülich
- ▶ *45th IFF Spring School 2014 "Computing Solids: Models, Ab-initio Methods and Supercomputing"* Mar 2014
Forschungszentrum Jülich
- ▶ *International Summer School "Fundamental Problems in Statistical Physics XIII"* Jun 2013
KU Leuven