



TO MAGNIFICO RETTORE OF UNIVERSITA' DEGLI STUDI DI MILANO

I the undersigned asks to participate in the public selection, for qualifications and examinations, for the awarding of a type B post-doc fellowship

Pavel Zolotarev

CURRICULUM VITAE

PERSONAL INFORMATION

Surname	Zolotarev
Name	Pavel
Date of birth	23.09.1992

PRESENT OCCUPATION

Appointment	Structure
Junior Data Scientist	Quantori (https://quantori.com/)

EDUCATION AND TRAINING

Degree	Course of studies	University	year of achievement of the degree
Diploma (= Laura Magistrale)	Physical Chemistry	Samara State University	2014
PhD	Crystal Chemistry	Samara State Technical University	2018

FOREIGN LANGUAGES

Languages	level of knowledge
English	Intermediate
German	Elementary
Italian	Elementary

AWARDS, ACKNOWLEDGEMENTS, SCHOLARSHIPS

Year	Description of award
2019	Best report in the condensed matter physics section on the XXIII International Scientific Conference of Young Scientists and Specialists (AYSS-2019), Dubna, Russia (application of topological analysis of procrystal electron densities as a tool for computational modeling of solid electrolytes)



2017	Samara Region "Young Scientist" Award (investigation of the organic molecular crystals suitable for application in organic molecular beam epitaxy)
------	--

TRAINING OR RESEARCH ACTIVITY

- Investigation of relationships between molecular structure, crystal structure and mechanical properties of hydrogen-bonded molecular crystals with quantum-mechanical (VASP) and topological methods (ToposPro) - Crystal structure analysis and modelling of adsorption properties of MOFs - Investigation of disordering and doping effects in cathode materials and solid electrolytes - Employment of exploratory data analysis and machine learning methods in solving materials science problems - Quantum-chemical modeling of molecules and crystalline solids (VASP, Gaussian09, CP2K) - Participation in international scientific collaborations (Russia, Germany, Italy, Iran, Argentina) - Presenting results of studies at international scientific conferences (Russia, UK, Spain, Croatia) - Writing scientific papers, applying for research grants, mentoring students, instructing at scientific schools and workshops
--

PROJECT ACTIVITY

Year	Project
2019-2021	Leader of the Russian Science Foundation grant "Influence of the physico-chemical properties of solvents on polymorphism of organic crystals" (project 19-73-00156)

CONGRESSES AND SEMINARS

Date	Title	Place
April 15-19, 2019	A combined approach for solid electrolytes investigations: handling geometrical/topological screening datasets	XXIII International Scientific Conference of Young Scientists and Specialists (AYSS-2019), Dubna, Russia
April 23-27, 2018	A topology-based investigation of the Ti-doping effects on the K ⁺ conductivity in doped K(Fe,Ti)O ₂ solid electrolyte	XXII International Scientific Conference of Young Scientists and Specialists (AYSS-2018), Dubna, Russia
October 2-6, 2017	Description of the NCA cathode material configurational space and elucidation of the dopants role in the structural stabilization	XXI International Scientific Conference of Young Scientists and Specialists (AYSS-2017), Dubna, Russia
May 30 - June 3, 2016	Identification of the cleavage planes in molecular crystals: topological and energetic aspects	8th National Crystallochemical Congress, Suzdal, Russia
August 23-28, 2015	Identification of the cleavage planes in molecular crystals: topological and energetic aspects	29th European crystallographic meeting (ECM29), Rovinj, Croatia



PUBLICATIONS

Articles in journals
"Relationships between Changes in Guest Ion Properties and in the Host Framework Topology in Ionic Coordination Polymers" Pavel N. Zolotarev, <i>Crystal Growth & Design</i> 2021, 21, 4959-4970 https://pubs.acs.org/doi/abs/10.1021/acs.cgd.1c00405
"On the Influence of Solvent Properties on the Structural Characteristics of Molecular Crystal Polymorphs" Pavel N. Zolotarev, Nadezhda A. Nekrasova <i>Crystal Growth & Design</i> 2020, 20, 7152-7162 https://doi.org/10.1021/acs.cgd.0c00753
"Ionic Transport in Doped Solid Electrolytes by Means of DFT Modeling and ML Approaches: A Case Study of Ti-Doped KFeO ₂ " Roman A. Eremin, Pavel N. Zolotarev, Andrey A. Golov, Nadezhda A. Nekrasova, Tilmann Leisegang <i>The Journal of Physical Chemistry C</i> 2019, 123, 29533-29542 https://doi.org/10.1021/acs.jpcc.9b07535
"Topological study of diverse hydrogen-bonded patterns found in a system of a nickel (II) complex and the sulfate anion" Miguel Angel Harvey, Sebastián Suarez, Pavel N. Zolotarev, Davide M. Proserpio, Ricardo Baggio <i>Acta Crystallographica Section C: Structural Chemistry</i> 2018, 74, 351-359 https://doi.org/10.1107/S2053229618002413
"Li(Ni,Co,Al)O ₂ Cathode Delithiation: A Combination of Topological Analysis, Density Functional Theory, Neutron Diffraction, and Machine Learning Techniques" Roman A. Eremin, Pavel N. Zolotarev, Olga Yu. Ivanshina, Ivan A. Bobrikov <i>The Journal of Physical Chemistry C</i> 2017, 121, 28293-28305 https://doi.org/10.1021/acs.jpcc.7b09760
"A 3D Coordination Network Built from CuII4Cl3(H ₂ O) ₂ Linear Clusters and Tetrapyridyl Tetrahedral Silane Ligands: Reversible Iodine Uptake and Friedel-Crafts Alkylation Reactions" Mahesh S. Deshmukh, Atul Chaudhary, Pavel N. Zolotarev, Ramamoorthy Boomishankar <i>Inorganic Chemistry</i> 2017, 56, 11762-11767 https://doi.org/10.1021/acs.inorgchem.7b01781
"Knowledge-Based Approaches to H-Bonding Patterns in Heterocycle-1-Carbohydrazonamide" Anna V. Vologzhanina, Andrey V. Sokolov, Pavel N. Zolotarev, Petr P. Purygin, Vladislav A. Blatov <i>Crystal Growth & Design</i> 2016, 16, 6354-6362 https://doi.org/10.1021/acs.cgd.6b00990
"Searching New Crystalline Substrates for OMBE: Topological and Energetic Aspects of Cleavable Organic Crystals" Pavel N. Zolotarev, Davide M. Proserpio, Massimo Moret, Silvia Rizzato <i>Crystal Growth & Design</i> 2016, 16, 1572-1582 https://doi.org/10.1021/acs.cgd.5b01695
"Synthesis and description of intermolecular interactions in new sulfonamide derivatives of tranexamic acid" M. Ashfaq, M.N. Arshad, M. Danish, A.M. Asiri, S. Khatoon, G. Mustafa, P.N. Zolotarev, R.A. Butt, O. Şahin, <i>Journal of Molecular Structure</i> 2016, 1103, 271-280 https://doi.org/10.1016/j.molstruc.2015.09.022
"A possible route toward expert systems in supramolecular chemistry: 2-periodic H-bond patterns in molecular crystals " Pavel N. Zolotarev, Muhammad Nadeem Arshad, Abdullah M. Asiri, Zahra M. Al-amshany, Vladislav A. Blatov <i>Crystal Growth & Design</i> 2014, 14, 1938-1949 https://doi.org/10.1021/cg500066p

Congress proceedings
"A machine learning approach for predicting formation enthalpy: A case study of Mackay-type approximants of icosahedral quasicrystals" Roman A. Eremin, Pavel N. Zolotarev, Tilmann Leisegang, Pavlo Solokha, AIP Conference Proceedings 2163 (1), 020003, AYSS-2019, Dubna, Russia, 2019
"Topological analysis of procrystal electron densities as a tool for computational modeling of solid electrolytes: A case study of known and promising potassium conductors" Pavel N. Zolotarev, Andrey A. Golov, Nadezhda A. Nekrasova, Roman A. Eremin AIP Conference Proceedings 2163 (1), 020007, AYSS-2019, Dubna, Russia, 2019



"A combined DFT/topological analysis approach for modeling disordered solid electrolytes" Pavel N. Zolotarev, NAdezhda A. Nekrasova, Andrey A. Golov, Roman A. Eremin, EPJ Web of Conferences 201, 02005, AYSS-2018, Dubna, Russia, 2018
"Comparative analysis of DFT-vdW vs. Coulomb energies for configurational space of layered cathode material at different delithiation levels" Pavel N. Zolotarev, Roman A. Eremin, EPJ Web of Conferences 201, 02004, AYSS-2018, Dubna, Russia, 2018
"Delithiated states of layered cathode materials: doping and dispersion interaction effects on the structure" Roman A. Eremin, Pavel N. Zolotarev, Ivan A. Bobrikov EPJ Web of Conferences 2018, 177, 02001, AYSS-2017, Dubna, Russia, 2017
"Topology-based description of the NCA cathode configurational space and an approach of its effective reduction" Pavel N. Zolotarev, Roman A. Eremin EPJ Web of Conferences 2018, 177, 02005, AYSS-2017, Dubna, Russia, 2017
"Identification of the cleavage planes in molecular crystals: topological and energetic aspects", PN Zolotarev, M Moret, DM Proserpio, Acta Crystallographica Section A: Foundations and Advances 71, s126-s127, 2015, ECM29, Rovinj, Croatia, 2013
"A topological study of three-dimensional hydrogen-bonded frameworks", PN Zolotarev, VA Blatov, Acta Crystallographica Section A: Foundations and Advances 69, s484, ECM28, Warwick, UK, 2013

Declarations given in the present curriculum must be considered released according to art. 46 and 47 of DPR n. 445/2000.

The present curriculum does not contain confidential and legal information according to art. 4, paragraph 1, points d) and e) of D.Lgs. 30.06.2003 n. 196.

Place and date: Samara, 14.04.2022

SIGNATURE