



AL MAGNIFICO RETTORE
DELL'UNIVERSITÀ DEGLI STUDI DI MILANO

COD. ID: 6763

Il sottoscritto chiede di essere ammesso a partecipare alla selezione pubblica, per titoli ed esami, per il conferimento di un assegno di ricerca presso il Dipartimento di Chimica

Responsabile scientifico: Prof. Pieraccini Stefano

Pavel Zolotarev

CURRICULUM VITAE

INFORMAZIONI PERSONALI

Cognome	Zolotarev
Nome	Pavel

OCCUPAZIONE ATTUALE

Incarico	Struttura
Assegnista di ricerca	Dipartimento di Chimica, Università degli Studi di Milano

ISTRUZIONE E FORMAZIONE

Titolo	Corso di studi	Università	anno conseguimento titolo
Laurea Magistrale o equivalente	Physical Chemistry	Samara State University	2014
Dottorato Di Ricerca	Crystal Chemistry	Samara State Technical University	2018

LINGUE STRANIERE CONOSCIUTE

lingue	livello di conoscenza
Inglese	C1
Italiano	A2

PREMI, RICONOSCIMENTI E BORSE DI STUDIO

anno	Descrizione premio
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)



ATTIVITÀ DI FORMAZIONE O DI RICERCA

descrizione dell'attività

February 2023 - Present

Research fellow Università degli Studi di Milano Statale, Milano, Italy

Conducting research on several topics:

- Application of bond valence theory to the search of potentially exfoliable inorganic materials, development of the code for carrying out screening of the large structural databases
- Collection and systematization of the hybrid organic-inorganic perovskites crystal structures, development of the ML model for prediction of the layers stacking in the layered lead-halogen perovskites depending on the nature of the organic cation
- Topological analysis of MD trajectories of crystals and liquids
- Topological analysis of the crystal structures of coordination polymers and MOFs
- Assistance in the organization of the conference and the workshop

August 2021 - January 2023

Data Scientist Quantori, Belgrade, Serbia

- Data preparation (cleaning, feature engineering, preparation of data loader), exploratory data analysis of the data from biomedical databases, classification and explainable ML, clustering, dimensionality reduction
- Participation in development of the custom data pipelines framework for the project
- Assistance to junior engineers, task assignment and review of their work
- Development of the code for running the MD simulation for estimation of the $\Delta\Delta G_{\text{binding}}$ in the protein-protein complexes upon substitutions of the amino acids in the chains

June 2013 - April 2022

Researcher Samara Center for Theoretical Materials Science (SCTMS), Samara State Technical University, Samara, Russia

- Investigation of relationships between molecular structure, crystal structure and mechanical properties of hydrogen-bonded molecular crystals
- 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
- Participation in international scientific collaborations (Russia, Germany, Italy, Iran, Argentina), presentation of results at international scientific conferences (Russia, UK, Spain, Croatia)
- Writing scientific papers, research grants application and leadership, mentoring students, instructing at scientific schools and workshops

ATTIVITÀ PROGETTUALE

Anno	Progetto
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)

CONGRESSI, CONVEGNI E SEMINARI

Data	Titolo	Sede
Agosto 26-30, 2024	A tool for the analysis of the bond strength anisotropy and search for the low-periodic substructures in crystalline solids	34th European crystallographic meeting (ECM34), Padova, Italia
Aprile 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
Aprile 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
Ottobre 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
Maggio 30 - Giugno 3, 2016	Identification of the cleavage planes in molecular crystals: topological and energetic aspects	8th National Crystallochemical Congress, Suzdal, Russia
Agosto 23-28, 2015	Identification of the cleavage planes in molecular crystals: topological and energetic aspects	29th European crystallographic meeting (ECM29), Rovinj, Croatia

PUBBLICAZIONI

Articoli su riviste
“A redox active rod coordination polymer from tetrakis(4-carboxylic acid biphenyl)tetrathiafulvalene” N. Zigon, F. Solano, P. Auban-Senzier, S. Grolleau, T. Devic, P.N. Zolotarev, D.M. Proserpio, B. Barszcz, I. Olejniczak, N. Avarvari, Dalton Transactions. 2024, 53, 4805-4813 https://doi.org/10.1039/D3DT04280D



"Relationships between Changes in Guest Ion Properties and in the Host Framework Topology in Ionic Coordination Polymers" Pavel N. Zolotarev, *Crystal Growth & Design* 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 *Crystal Growth & Design* 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 KFeO₂" Roman A. Eremin, Pavel N. Zolotarev, Andrey A. Golov, Nadezhda A. Nekrasova, Tilmann Leisegang *The Journal of Physical Chemistry C* 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 *Acta Crystallographica Section C: Structural Chemistry* 2018, 74, 351-359 <https://doi.org/10.1107/S2053229618002413>

"Li(Ni,Co,Al)O₂ 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 *The Journal of Physical Chemistry C* 2017, 121, 28293-28305 <https://doi.org/10.1021/acs.jpcc.7b09760>

"A 3D Coordination Network Built from CuII4Cl3(H₂O)₂ Linear Clusters and Tetrapyrindyl Tetrahedral Silane Ligands: Reversible Iodine Uptake and Friedel-Crafts Alkylation Reactions" Mahesh S. Deshmukh, Atul Chaudhary, Pavel N. Zolotarev, Ramamoorthy Boomishankar *Inorganic Chemistry* 2017, 56, 11762-11767 <https://doi.org/10.1021/acs.inorgchem.7b01781>

"Knowledge-Based Approaches to H-Bonding Patterns in Heterocycle-1-Carbohydrazonamides" Anna V. Vologzhanina, Andrey V. Sokolov, Pavel N. Zolotarev, Petr P. Purygin, Vladislav A. Blatov *Crystal Growth & Design* 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 *Crystal Growth & Design* 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, *Journal of Molecular Structure* 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 *Crystal Growth & Design* 2014, 14, 1938-1949 <https://doi.org/10.1021/cg500066p>

Atti di convegni

- "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

ALTRE INFORMAZIONI

Google Scholar	https://scholar.google.ru/citations?user=IGMhJS8AAAAJ&hl=en
LinkedIn	https://www.linkedin.com/in/pavel-n-zolotarev/
GitHub	https://github.com/trioxane/

Le dichiarazioni rese nel presente curriculum sono da ritenersi rilasciate ai sensi degli artt. 46 e 47 del DPR n. 445/2000.

Il presente curriculum, non contiene dati sensibili e dati giudiziari di cui all'art. 4, comma 1, lettere d) ed e) del D.Lgs. 30.6.2003 n. 196.

RICORDIAMO che i curricula **SARANNO RESI PUBBLICI sul sito di Ateneo** e pertanto si prega di non inserire dati sensibili e personali. Il presente modello è già pre-costruito per soddisfare la necessità di pubblicazione senza dati sensibili.

Si prega pertanto di **NON FIRMARE** il presente modello.

Luogo e data: Milano, 01.09.2024