Phone: (012) 295 28 15, Fax: (012) 2952804, room: 208B
e-mail: trybulamarcela@wp.eu, m.trybula@imim pl
Employment and positions
Institute of Metallurgy and Materials Science, Polish Academy of Sciences: assistant professor (from 10.2017 - 11.2023)
University of Warsaw Biological and Chemical Research Centre: assistant professor (since 2020-2022)
Institute of Metallurgy and Materials Science, Polish Academy of Sciences: associate professor (from 12.2023 - present)
Scientific career
M.Sc.: Jagiellonian University, Faculty of Chemistry, 2010

Ph.D.: Institute of Metallurgy and Materials Science PAS, 2015
Habilitation: Institute of Metallurgy and Materials Science PAS, 2023
Scientific achievements
ORCID: https://orcid.org/0000-0003-4802-9200
The most relevant publications during last 5 years
1. 1.
<b>Marcela E. Trybula</b> , Przemysław W. Szafrański and Pavel A. Korzhavyi "Structure and chemistry of liquid Al-Cu alloys: molecular dynamics study versus thermodynamics-based modelling", J. Mater. Sci., 11 (2018) 8285-8301.
2.
Marcela E. Trybula, Sylwia Terlicka, Przemyslaw Fima "Thermodynamics of liquid Li-Sb alloys - Experiment vs modeling" J. Chem. Therm., 128 (2019) 134-140.
3.
Patryk Kasza, <b>Marcela E. Trybula</b> , Katarzyna Baradziej, Przemysław W. Szafrański, Marek Cegła. "Fluorescent triazolyl spirooxazolidines: Synthesis and NMR stereochemical studies"

J. Mol. Str., 1183 (2019) 157-167.

4.

**Marcela E. Trybula** and Pavel A. Korzhavyi " Atomistic Simulations of Al(100) and Al(111) Surface Oxidation: Chemical and Topological Aspects of the Oxide Structure", J. Phys. Chem. C, 123, 1, (2019) 334-346.

5.

P.W. Szafrański, **M.E. Trybula**, P. Kasza, M.T. Cegła, "Following the oxidation state of organosulfur compounds with NMR: Experimental data versus DFT calculations and database-powered NMR prediction" J. Mol. Str., 1202 (2020) 157-167.

6.

Aleksandra Drewienkiewicz, Arkadiusz Żydek, **Marcela E. Trybula** and Janusz Pstruś "Atomic Level Insight into Wetting and Structure of Ag Droplet on Graphene Coated Copper Substrate-Molecular Dynamics versus Experiment", Nanomaterials, 11(6), 2021, 1465, 1465: 1-16.

7.

Arkadiusz Żydek, Mariusz Wermiński and **Marcela E. Trybula** " Description of grain boundary structure and topology in nanocrystalline aluminum using Voronoi analysis and order parameter" Computational Materials Science, Volume 197, (2021) 110660:1-12.

8.

**Marcela E. Trybula** and Pavel A. Korzhavyi " Atomistic Simulations of Al(100) and Al(111) Surface Oxidation: Chemical and Topological Aspects of the Oxide Structure", Journal of Physical Chemistry C, 123, 1, (2019) 334-346.

9.

**Marcela E. Trybula** and Pavel A. Korzhavyi "Temperature dependency of structure and order evolution in 2D confined oxide films grown on Al substrates using reactive molecular dynamics", Vacuum, 190, (2021) 110243:1-8.

10.

**Marcela E. Trybula**, Arkadiusz Żydek, Pavel Korzhavyi, Joanna Wojewoda-Budka "Structure and behaviour of oxide-coated aluminum surface in contact with strongly alkaline and acidic aqueous solutions - a reactive molecular dynamics simulation study" Journal of Physical Chemistry C, 127 (5), (2023), 2493-2507

### **Research Projects**

# **NSC Projects**

Thermodynamic and physical properties of liquid binary alloys, PRELUDIUM, 2011/03/N/ST8/05308 - principal investigator (08.2012-08.2014)

Thermodynamic, structural and physicochemical properties of liquid Al.-Li-Zn alloys, ETIUDA, 2014/12/T/ST8/00089 - principal investigator (10.2014- 06.2015)

Mechanism of the discontinuous precipitation reaction - an atomistic simulation study, SONATA,

Experience gained abroad

NCN2016/21/D/ST8/01689 - principal investigator (10.2017-10.3019)
Thermodynamic and structural properties of liquid Ag-Li-Sb alloys, OPUS, NCN2015/19/B/ST8/0107 - investigator (07.2016 - 09.2017)
- Mass transport processes in phase transformations at moving boundaries of discontinuous precipitates-experiment vs. modelling, OPUS, 2017/25/B/ST8/02198 - investigator (03.2020-12.2020)
European Union and other Projects
Innovative and affordable service for the Preventive Conservation monitoring of individual Cultural Artefacts during display, storage, handling and transport, CollectionCare project, Horizon2020, 501-D31260-0534653 - investigator, (03.2020-01.2022)
ALUminium oXides for processing and products, ALUX, Swedish Foundation for Strategic Research (SSF), RMA11-0090 - investigator, (01.2017-12.2018)

<del>-</del>
Institute of Technology in Grenoble, Grenoble, France, 2014-2015 (4 months)
<del>-</del>
Physical Properties of Materials, Research with Neutrons and Muons Division, Paul Scherrer Institute, Villigen, Switzerland, 2015 (1 week)
<del>-</del>
School of Chemical Technology, Aalto University, Aalto, Finland, 2015 (1 week)
-
KTH Royal Institute of Technology, Stockholm, Sweden, 2017-2018 (24 months)
Prizes and awards
Prizes and awards
Prizes and awards
Prizes and awards  - 2014 ETIUDA Doctoral scholarship
<del>-</del>
<del>-</del>
- 2014 ETIUDA Doctoral scholarship -
- 2014 ETIUDA Doctoral scholarship -
- 2014 ETIUDA Doctoral scholarship  - 2015 Larry Kauffman Scholarship  -

-
2020 - 3 year fellowship for outstanding young scientists granted by Ministry of Science and Higher Education
7.07.2015 invited seminar, Condensed Matter Theory Group at PSI, Villigen, Switzerland, entitled: "Multiscale Description of structural and thermophysical properties of liquid alloys"
Education of scientific staff
Supervisor of Master thesis: Arkadiusz Żydek, University of Technology AGH, 2020, "Impact o Grain Boundary Complexion on structural properties in aluminum alloy"
Co-supervisor of PhD thesis: Monika Bugajska Institute of Metallurgy and Materials Science, PAS, 2020, "Thermodynamic properties of liquid Ag-Li-Sb alloys"
Supervisor of internshipers:
Students from Jagiellonian University and University of Technology AGH, 2017-2019
3-months internships of ERASMUS+ student at KTH Royal Institute of Technology, Sweden, 2017

Intern	ational	COOL	peration
	ational		JU: 41.U:

Department of Materials Science and Engineering, KTH Royal Institute of Technology, Stockholm, Sweden - Prof. Pavel Korzhavyi

# Organisation of conferences and scientific events

Co-organizator of discussion panel M8: Predicting Interface Structure and Dynamics - From Atomic- to Meso-Scale Materials Science and Engineering Congress (MSE) Darmstadt, Germany, 25.09-27.09.2018

Co-organizator of discussion panel M16: Predicting Interface Structure and Dynamics - From Atomic- to Meso-Scale Materials Science and Engineering Congress (MSE) Darmstadt, Germany, 22.09.- 25.09.2020

Co-organizator of discussion panel M01: Interfaces in Advanced Materials: From Atomistic - to Meso-Scale Materials Science and Engineering Congress (MSE) Darmstadt, Germany, 27.09.-29.09.2022

#### Membership in professional societies

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Member of Discussion Panel of Crystals MDPI, 2020

#### Main areas of scientific interests

Structure and properties of liquid aluminum based alloys, thin films and grain boundary studies of manocrystalline and polycrystalline aluminum and its alloys at the nanoscale, computational materials science (molecular dynamics, Monte Carlo, DFT calculations, Voronoi polyhedral analysis), semi-empirical modelling