

Izabela Czekaj



Academic degrees : doctor habilitatus in Engineering

Position : Professor of CUT

Engineering - technical field

Discipline Chemical engineering

Academic qualifications:

University teacher (molecular modeling, experimental methods, organic nitrogen compounds, heterogeneous catalysis, environmental protection legislation, organic technology, urea technology), member of the Scientific Council of the Faculty of Chemical Engineering and Technology of the Cracow University of Technology

Membership in professional and academic boards :

Member of the Polish Chemical Society, Expert of the EU Horizon 2020 programs and the Polish NCBiR

Academic merits :

Prof Czekaj has several years experience in scientific work abroad (Switzerland, Paul Scherrer Institute 2005-2013, ETH Zurich 2013-2014) and published 40 articles/books in international peer reviewed journals, which are cited more than 1062 (Scopus) and 1395 (Google Scholar). Her h-index is 17 (Scopus) and 20 (Google Scholar). Selected publications: 1. N. Sobuś, et al., and I. Czekaj, Design of Co, Cu and Fe-BEA zeolite catalysts for selective conversion of lactic acid into acrylic acid, *Catalysis Letters*, 149 (2019), 3349-3360. doi: 10.1007/s10562-019-02883-8. 2. P. Zaręba, J. Jaśkowska, I. Czekaj, G. Satała, New Halogen-substituted Arylpiperazine Derivatives of Naphtholactam and Naphthosultam. Development of Ecological Synthesis, *Bioorganic & Medicinal Chemistry* 27 (2019) 3396-3407. doi: 10.1021/jm10022923. Izabela Czekaj, Natalia Sobuś, Vibrational structure of selected compounds derived from biomass: lignin dimers, selected aldopentoses and aldohexoses, *Journal of Chemistry and Chemical Engineering* 12 (2018) 11-19. doi: 10.17265/1934-7375/2018.01.002 4. Leanza, C. A. F. Vaz, I. Czekaj, P. Novák, M. El Kazzi, Solving the puzzle of Li₄Ti₅O₁₂ surface reactivity in aprotic electrolytes in Li-ion batteries by nanoscale XPEEM spectromicroscopy, *Journal of Materials Chemistry A : materials for energy and sustainability* 6, 2018, 3534-3542. doi: 10.1039/C7TA09673A.5. M. Moser, I. Czekaj, N. Lopez, J. Perez-Ramirez, The virtue of defects: stable bromine production via catalytic oxidation of hydrogen bromide on titanium oxide, *Angew. Chem. Int. Ed.* 2014, 53, 1–6. doi: 10.1002/ange.201404022

Scientific projects: industrial project (with Casale) "Molecular Modelling for deNO_x" (1 PhD student); industrial project (with Zeocomplex, technologist) "Research and development of zeolite preparations for multiphase deodorization", 2020-2022; scientific project Polonez-1 Polish National Science Center under EU MSCA action „Nano-design of zeolite-based catalysts for selective conversion of biomass into chemicals” 2015/19/P/ST4/02482 (1 PhD student), 2016-2018; scientific project sponsored by Swiss National Foundation „Computational modeling of Pd/PdOx transformation in redox catalytic cycles” 200021-116184 (1 PhD student, 1 postdoc), 2008-2012.

Professional qualifications/language skills

Habilitated doctor in technical sciences in the discipline of chemical technology, Doctor of chemical sciences in chemistry, Master of Science in the field of specialization Engineering of technological processes Knowledge of foreign languages: Polish (fluent), English (fluent), German (advanced)

Research field :

Prof. Czekaj is a computational chemist, chemical engineer, technologist and material scientist with strong interest in the design of chemical/electronic and catalytic/adsorption properties of nanomaterials, and in their application in electrochemistry, optoelectronic devices, catalysis and organic technology. Important expertise of her group "Catalytic and Nanostructured Materials Design" is the theoretical modeling and characterization of nanomaterials and catalysts electronic structure, synthesis, design and physicochemical characterisation of materials, experimental design of innovative technological processes as well as scale-up to industrial level. She is interested in: Experimental and theoretical investigations of innovative catalysts and materials for organic technology processes. Molecular modeling of materials for catalysis and electrocatalysis, energy generation and storage, adsorption. Design of materials for lignocellulosic biomass valorization, selective catalytic reduction deNO_x

processes, odor reduction, catalysts for CO₂ catalytic reduction processes, methanation of biomass-derived synthesis gas. Materials: transition metal oxides, halide perovskite nanocrystals for next generation optoelectronic and photonic technologies, metal organic frameworks, synthetic and natural zeolites for catalysis and adsorption processes.

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Useful links :

<http://zeodesign-polonez.pk.edu.pl/>