POLISH NATIONAL AGENCY FOR ACADEMIC EXCHANGE

STER PROGRAMME

name of the unit:		symbol:
RESEARCH GROUP OF SOLUTION PHYSICAL CHEMISTRY Institute of Applied Radiation Chemistry, Lodz University of Technology		I-34 http://www.mitr.p.lodz.pl
head of the unit:	potential promoters:	contact person:
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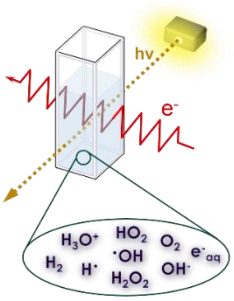
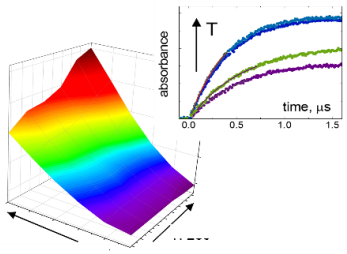
scope of activities:

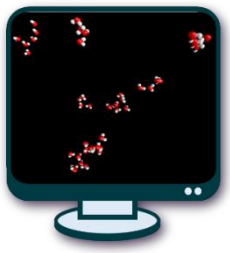
Computer simulation and pulse-radiolysis measurement based research addressing the energy deposition and impact of ionizing radiation on aqueous solutions, mechanistic understanding of high-temperature water radiolysis, solvent effects on properties and reactions of transient radical species, analysis of hydrogen bonding interaction, ion solvation in binary solvents.



Present and future activities:

- Molecular dynamics simulation based study of hydrogen bonding and solvent effects in aqueous systems at ambient and supercritical conditions.
- Kinetic studies of transient radical species in binary aqueous solutions.
- Mechanistic understanding of high-temperature water radiolysis.
- Interdisciplinary basic research supporting the nuclear energy applications, including:
  - numerical simulation of LWR coolant chemistry,
  - analysis of hydrogen generation,
  -development of methods for controlling oxidising environment.





Selected representative publications (2014-2022):

D. Swiatla-Wojcik, A Numerical Simulation of Radiation Chemistry for Controlling the Oxidising Environment in Water-Cooled Nuclear Power Reactors, Appl. Sci. 12 (2022) 947.

A. Lewandowska-Andralojc, G.L. Hug, B. Marciniak, G. Horner, D. Swiatla-Wojcik, Water-Triggered Photoinduced Electron Transfer in Acetonitrile-Water Binary Solvent. Microstructure-Tuned Reactivity of Hydrophobic Solutes. J. Phys. Chem. B 124 (2020) 5654.

D. Swiatla-Wojcik, J. Szala-Bilnik, High Temperature Aqueous Solvent Effect on Stretching Vibrations of the Hydroxyl Radical – MD Simulation Study of Spectral Shifts and Hydrogen Bond Statistics. J. Supercrit. Fluids 143 (2019) 126.

D. Swiatla-Wojcik, J. Szala-Bilnik, High Temperature Aqueous Solvent Effect on Translational and Hydrogen Bond Dynamics of the Hydroxyl Radical — MD Simulation Study. J. Supercrit. Fluids 145 (2019) 103.

L. Kazmierczak, M. Wolszczak, D. Swiatla-Wojcik, Ionic-Equilibrium-Based Mechanism of ·OH Conversion to Dichloride Radical Anion in Aqueous Acidic Solutions by Kinetic and Theoretical Studies. J. Phys. Chem. B 123 (2019) 528.

L. Kazmierczak, D. Swiatla-Wojcik, M. Wolszczak, Rate of Reaction of the Hydrogen Atom with Nitrous Oxide RSC Advances. 7 (2017) 8800.

D. Swiatla-Wojcik, Water-Structure Based Mechanistic View on the Bimolecular Decay of the Hydrated Electron, Chem. Phys. Lett. 641 (2015) 51.

D. Swiatla-Wojcik, A. Mozumder, Assessment of Hydrogen Bonding Effect on Ionization of Water from Ambient to Supercritical Region - MD Simulation Approach Radiat. Phys. Chem. 97 (2014) 113.

Keywords:
Solvent effects, hydrogen bonding, binary solvents, high-temperature water radiolysis, molecular simulation, kinetic simulation, reaction kinetics, supercritical water

List of internship proposal in this research team:

Kinetic simulation of complex chemical systems. A traineeship is related to the computational chemical kinetics and concerns numerical simulation and kinetic analysis of multi-reactant systems.