Synchrotron Radiation Techniques
for Catalysts and Functional Materials

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ABSTRACTS

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Federal Research Center Boreskov Institute of Catalysis
Synchrotron Radiation Facility SKIF
Budker Institute of Nuclear Physics of SB RAS
Novosibirsk State University

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Сборник включает тезисы пленарных, устных и стендовых докладов.
Основные темы научной программы конференции:
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- Theoretical and applied aspects of experimental techniques utilizing synchrotron radiation
- Structure-driven design of catalysts and functional materials based on synchrotron diagnostics
- Synchrotron radiation for structural biology
- Development of instrumentation for synchrotron beamlines
- New data processing algorithms, artificial intelligence and machine learning in bulk data analysis

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Structural Biology in the Study of Enzyme Catalysis: An Example of DNA Glycosylases

Zharkov D.O.[1,2]

1 – Novosibirsk State University, Novosibirsk, Russia

2 – SB RAS Institute of Chemical Biology and Fundamental Medicine, Novosibirsk, Russia

dzharkov@niboch.nsc.ru

About 100,000 nucleotides in DNA in each cell of the human body are damaged daily by a variety of endogenous and environmental factors. To prevent mutations and cell death, several enzymatic DNA repair systems had evolved. The most common types of DNA lesions, such as products of oxidation, deamination, and alkylation, are removed by base excision repair. This process is initiated by DNA glycosylases, the enzymes that hydrolyze the *N*-glycosidic bond of the damaged deoxyribonucleotide. All living species have several DNA glycosylases with different substrate specificities; e. g., eleven DNA glycosylases are currently known from human cells, and nine, in *Escherichia coli*. Based on their sequences and three-dimensional structures, DNA glycosylases can be divided into several unrelated superfamilies. However, some DNA glycosylases belonging to different superfamilies can have identical substrate specificities. The question of how DNA glycosylases discriminate between substrate and nonsubstrate nucleobases has not yet been resolved. The structures of many DNA glycosylases and their complexes with DNA has been determined by X-ray crystallography and NMR spectroscopy. A number of modified nucleotides has been synthesized, allowing one to analyze the features of damaged base recognition. Modern approaches to studying the mechanisms of damage recognition by DNA glycosylases are based on a combination of complementary structural, computational and biochemical methods, making it possible to establish the principles of selection of damaged nucleobases among a large excess of normal ones, based on multiple conformational transitions during the recognition process.

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