ANDREY KOVALEVSKY, Ph.D.

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SCIENTIST with proficiency in biochemistry, structural biology, structure-based drug design, funding acquisition, project management, and personnel supervision.
Research statement: Studying protein structure, dynamics and function, enzyme mechanisms and performing structure-assisted design of antivirals and anticancer drugs.
Achievements: >200 peer-reviewed publications, >7000 citations, 9 funded grants, *h* index 51.
Multilingual: English, Russian, Ukrainian.

AREAS OF EXPERTISE

- Structural biology
- X-ray/neutron crystallography
- Biomolecular Assays
- Macromolecular crystal growth
- Biochemistry and biophysics
- Protein expression/purification
- Biomolecular modeling
- Quantum chemistry
- Oral/Written Communication
- Team leadership and supervision
- Project management
- Funding acquisition

EDUCATION & TRAINING

Postdoctoral Fellow 2007-2010
Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM
Postdoctoral Associate 2004-2007
Department of Biology, Georgia State University, Atlanta, GA
Postdoctoral Associate 2003-2004
Department of Chemistry, University at Buffalo, the State University of New York, Buffalo, NY
Ph.D. in Chemistry, 2003
Department of Chemistry, University at Buffalo, the State University of New York, Buffalo, NY
GPA: 3.972
M.S. with Honors in Chemistry 1996
Kharkov State University, Kharkov, Ukraine

FUNDING

- NIH R21 NS120839, 2022-2024 ($500K).
- NIH R01 GM137008, 2020-2024 ($2.8M).
- NIH U01 NS083451, 2014-2019 ($2.6M).
- ORNL Neutron Sciences Directorate Science Initiative Postdoctoral program, 2020-2023 ($500K).
- ORNL Neutron Sciences Directorate GO! PhD student program, 2016-2019 ($180K).
- ORNL LDRD, 2011-2013 ($400K); 2014-2015 ($180K).
- DOE-BER, 2012-2013 ($400K).
- LANL LDRD, 2011-2014 ($1M).
- LANL Director's Postdoctoral Fellowship 2008-2010 ($300K).

PATENTS

- Radic et al., US Patent 11,820,749 B2, Centrally active and orally bioavailable uncharged bisoxime antidotes for organophosphate poisoning and methods for making and using them. Issued 11/21/2023.

SPECIAL HONORS / ENGAGEMENTS

- Secretary of Energy Achievement Award to National Virtual Biotechnology Laboratory, 2020.
- UT-Battelle Research Accomplishment Award, ORNL, 2020.
- HFSP Nakasone Award Nominee, 2020.
- Blavatnik Awards for Young Scientists Nominee from ORNL, 2014.
- Postdoctoral Distinguished Performance Award, LANL 2009.
- Director's Postdoctoral Fellow, LANL 2008-2010.
- Silbert Graduate Fellowship, Chemistry Department, SUNY Buffalo, 2002-2003.
- Pauling Prize, ACA Annual Meeting, San Antonio TX, 2002.
- International Soros Science Education Program Award, Moscow, Russia, 1998.

PROFESSIONAL EXPERIENCE

DISTINGUISHED R&D SCIENTIST – *Neutron Scattering Division, ORNL, Oak Ridge, TN*
(2023 – current)
SENIOR R&D SCIENTIST – *Neutron Scattering Division, Oak Ridge National Laboratory, Oak Ridge, TN*
(2018 – 2023)
R&D SCIENTIST 3 – *Biology and Soft Matter Division, Oak Ridge National Laboratory, Oak Ridge, TN*
(2012 – 2018)

- Managed and led NIH- and DOE-funded research projects, including structure-dynamics-function studies of viral proteases (SARS-CoV-2, norovirus, dengue virus, HIV-1), vitamin B_6-dependent enzymes, design of oxime reactivators of organophosphate-inhibited human acetylcholinesterase, design of SARS-CoV-2 main protease inhibitors, and design of anticancer drugs targeting metabolic enzymes. Designed and implemented strategies in joint X-ray/neutron protein crystallography, protein deuteration, purification and crystallization, and biomolecular simulations. Developed joint neutron/MD sub-THz vibrational spectroscopy to study protein vibrational dynamics effects on substrate and inhibitor binding to proteins. Supervised research scientists, postdoctoral associates, and students. Managed an X-ray crystallography/BioSAXS lab and IMAGINE/MaNDi neutron diffraction instrument suite. Prepared grant proposals to NIH and DOE. Prepared patent applications.

R&D SCIENTIST 2 – *Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM*
(2010 – 2012)

- Managed multidisciplinary collaborations and teams to create protein structure-function projects and secure funding. Used X-ray/neutron protein crystallography, enzyme kinetics, rational protein engineering and quantum-chemical calculations for mechanistic studies of enzymes and improved their performance by mutagenesis. Managed several concurrent research projects. Served as a Beamline Scientist at the neutron Protein Crystallography Station at LANSCE. Mentored and oversaw professional development of postdoctoral scientists and students.

POSTDOCTORAL FELLOW – *Bioscience Division, Los Alamos National Laboratory, Los Alamos, NM*
(2007 – 2010)

- Led studies of enzyme mechanisms and protein/ligand complexes by X-ray/neutron protein crystallography for rational drug design and protein engineering. Expressed, purified (in milligram-to-gram quantities) and crystallized deuterated proteins. Collected, refined, analyzed X-ray and neutron diffraction data. Operated robotic protein crystal growth instrumentation. Managed several concurrent research projects. Supervised research of graduate and undergraduate students. Acted as a Beamline Scientist at the neutron Protein Crystallography Station user facility.

POSTDOCTORAL ASSOCIATE – *Department of Biology, Georgia State University, Atlanta, GA*
(2004 – 2007)

- Spearheaded a team of postdoctoral researchers and students studying the molecular basis of HIV-1 protease drug resistance. Collected, solved and refined X-ray diffraction data. Analyzed high-resolution ligand-free and protein/ligand crystal structures. Expressed, purified, crystallized proteins. Studied enzyme kinetics and inhibition by UV-Vis and fluorescence spectroscopic assay methods. Performed site directed mutagenesis. Performed QM calculations.

POSTDOCTORAL ASSOCIATE – *Department of Chemistry, SUNY Buffalo, Buffalo, NY*
(2003 – 2004)

- Instrumental in designing and execution of the state-of-the-art time-resolved photo-crystallographic experiments. Obtained atomic structures of excited-state molecules in crystals. Synthesized and characterized transition metal complexes. Studied photo-induced charge transfer in the solid state using laser spectroscopy. Performed QM calculations of organic and inorganic molecules. Crystallized compounds utilizing a variety of methods. Collaborated with international research groups on the project studying conductive and magnetic properties of fullerene co-crystals with organic and inorganic compounds.

PHD STUDENT / RESEARCH ASSISTANT – *Department of Chemistry, SUNY Buffalo, Buffalo, NY*
(1999 – 2003)

- Designed and executed photo-crystallographic experiments. Obtained accurate molecular structures of photo-induced products in crystals of ruthenium complexes, characterized by FT-IR and DSC. Synthesized and characterized ruthenium and iron coordination and organometallic compounds. Performed QM calculations of organic and inorganic molecules. Crystallized a number of coordination compounds. Solved, refined and analyzed crystal structures for and communicated with various research groups as a Departmental Service Crystallographer.

RESEARCH ASSISTANT / SERVICE CRYSTALLOGRAPHER – *Chemical Crystallography Laboratory, Nesmeyanov Institute of Organoelement Compounds, Moscow, Russia*
(1996 – 1999)

- Synthesized and characterized organic heterocyclic compounds by spectroscopy and crystallography. Employed QM and MM calculations to study conformational flexibility of organic heterocyclic molecules. Extensively grew crystals and performed service crystallography.

AFFILIATIONS

Research Professor & Adjunct Graduate Faculty Member (2014 – current)
Department of Chemistry, University of Toledo, Toledo OH

Regular Faculty (2012 – current)
Faculty of 1000, Experimental Biophysical Methods Section, London, UK

Joint Faculty Associate Professor (2015 – 2020)
Department of Biochemistry & Cellular and Molecular Biology, University of Tennessee, Knoxville TN