ANDREY KOVALEVSKY, Ph.D.

Biology and Soft Matter Division ▪ 1 Bethel Valley Rd., P.O. Box 2008 ▪ Oak Ridge National Laboratory ▪ Oak Ridge, TN 37831-6475

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SCIENTIST with proficiency in structural biology, biochemistry, and molecular simulations.

Multilingual: English, Russian, Ukrainian.

AREAS OF EXPERTISE

- Project Management
- Team Leadership
- Macromolecular crystallography
- Protein Chemistry
- Protein expression, purification, crystallization, enzyme kinetics
- Small-angle scattering – SAXS, SANS
- UV-Vis, fluorescence, vibrational (IR, neutron) spectroscopies
- QM/MM/MD
- Oral / Written Communication

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 Physical Chemistry / Crystallography 2003
Department of Chemistry, University at Buffalo, the State University of New York, Buffalo, NY
GPA: 3.972

M.S. with Honors in Synthetic Organic Chemistry 1996
Kharkov State University, Kharkov, Ukraine

FUNDING

- NIH U01, 2014-2019, “Accelerated AChE reactivator design by mechanistic neutron scattering studies”.
- ORNL LDRD, 2014-2015, “Structure-function studies of nucleic acids using neutron crystallography enabled by selenium modification”.
- DOE-BER, 2012-2013, “Combining neutrons with high-performance computing to produce value-added products from lignocellulosic biomass”.
- LANL LDRD, 2011-2014, “Biofuel enzymes by design”.
- ORNL LDRD, 2011-2013, “Re-engineering xylanase”.
- LANL Director’s Postdoctoral Fellowship 2008-2010, “Determining the mechanisms of enzymes xylose isomerase and HIV protease using neutron crystallography”.

ACHIEVEMENTS

- 150 peer-reviewed publications, 20 invited talks and oral presentations, *h* index 32
- Journal covers: *Structure* 2010; *Angew. Chem. Int. Ed.* 2011; *Acta Crystallogr. D* 2014.
- Combining neutron crystallography with simulation for protein structure-function and drug design studies.
- First to directly observe hydronium ion, proton complexation and proton transfer in proteins.

SPECIAL HONORS / ENGAGEMENTS

- Blavatnik Awards for Young Scientists Nominee, 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

R&D SCIENTIST 3 – *Biology and Soft Matter Division, Oak Ridge National Laboratory, Oak Ridge TN (2012 – Present)*

- Managed research projects in mechanistic enzymology, protein engineering and drug design. Designed and implemented strategies in joint X-ray/neutron protein crystallography, enzyme kinetics, protein engineering, QM/MM calculations and MD simulations. Supervised postdoctoral associates, students, technologists. Led science thrusts for neutron diffractometers at SNS and HFIR.

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, 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, 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	MEMBERSHIPS
Research Professor & Adjunct Graduate Faculty Member (2014 – current) Department of Chemistry University of Toledo, Toledo OH	American Crystallographic Association (ACA) 2001 – current
Joint Faculty Associate Professor (2015 – current) Biochemistry & Cellular and Molecular Biology University of Tennessee, Knoxville TN	American Association for the Advancement of Science (AAAS) 2016 – current
Faculty Member (2012 – current) Faculty of 1000 Experimental Biophysical Methods Section	