

## **ANDREY KOVALEVSKY, Ph.D.**

Neutron Scattering Division ▪ Oak Ridge National Laboratory ▪ Oak Ridge, TN 37831-6475

PHONE: 505-310-4184 ▪ FAX: 865-574-2033 ▪ E-MAIL: [kovalevskyay@ornl.gov](mailto:kovalevskyay@ornl.gov)

[orcid.org/0000-0003-4459-9142](https://orcid.org/0000-0003-4459-9142) ▪ [www.ornl.gov/staff-profile/andrii-y-kovalevskiy](http://www.ornl.gov/staff-profile/andrii-y-kovalevskiy)

---

**SCIENTIST** with proficiency in biochemistry, structural biology, structure-based drug design, funding acquisition and project management.

**Research statement:** Studying protein structure, dynamics and function, performing rational drug design with joint x-ray/neutron crystallography, neutron vibrational spectroscopy, cryo-EM and biomolecular (and VR) modeling.

**Achievements:** >200 peer-reviewed publications, >7000 citations, 9 funded grants, *h* index 50.

**Multilingual:** English, Russian, Ukrainian.

### **AREAS OF EXPERTISE**

- |                                 |                                 |                                 |
|---------------------------------|---------------------------------|---------------------------------|
| - Structural biology            | Biochemistry and biophysics     | Oral/Written Communication      |
| - X-ray/neutron crystallography | Protein expression/purification | Team leadership and supervision |
| - Molecular spectroscopy        | Biomolecular modeling           | Project management              |
| - Macromolecular crystal growth | Virtual reality modeling        | 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**

- U.S. Patent Application 17/613775, Centrally active and orally bioavailable uncharged bisoxime antidotes for organophosphate poisoning and methods for making and using them.

### **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**

**SENIOR R&D SCIENTIST** – *Neutron Scattering Division, Oak Ridge National Laboratory, Oak Ridge, TN*  
(2018 – 2023)

- ❖ Managed and led NIH- and DOE-funded research projects in structural biology, including structure-dynamics-function studies of SARS-CoV-2 viral proteins, pyridoxal-5'-phosphate (PLP, vitamin B<sub>6</sub>)-dependent enzymes, design of oxime reactivators of organophosphate-inhibited human acetylcholinesterase and design of specific inhibitors of SARS-CoV-2 main protease. 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 beamlines.

**R&D SCIENTIST 3** – *Biology and Soft Matter Division, Oak Ridge National Laboratory, Oak Ridge, TN*  
(2012 – 2018)

- ❖ 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 research scientists, postdoctoral associates, students. Led science thrusts for neutron diffractometers at SNS and HFIR. Managed an X-ray crystallography/BioSAXS lab and IMAGINE neutron diffraction beamline.

**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