BIOGRAPHICAL SKETCH

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NAME: Ando, Nozomi

eRA COMMONS USER NAME (credential, e.g., agency login): nando1

POSITION TITLE: Associate Professor of Chemistry and Chemical Biology

EDUCATION/TRAINING *(Begin with baccalaureate or other initial professional education, such as nursing, include postdoctoral training and residency training if applicable. Add/delete rows as necessary.)*

INSTITUTION AND LOCATION	DEGREE *(if applicable)*	Completion Date MM/YYYY	FIELD OF STUDY
Massachusetts Institute of Technology	B.S.	06/01	Physics
Cornell University	M.S.	05/04	Physics
Cornell University	Ph.D.	01/09	Physics
Massachusetts Institute of Technology	Postdoctoral	06/14	Chemistry

A. Personal Statement

The focus of my research program is to understand the molecular mechanisms of protein allostery. To do so, my lab uses X-ray scattering, crystallography, cryo-electron microscopy (cryo-EM), and bioinformatics. We are best known for our innovations in X-ray scattering, which allows us to interpret conformational heterogeneity in terms of protein motions and structural rearrangements (*Chem Rev* 2017). This approach has allowed us to map the conformational landscape of allosteric enzymes and identify evolutionary patterns (*JACS* 2017, *PNAS* 2018, *Nature Comm* 2019). Most recently, we were the first to solve a long-standing problem in X-ray crystallography by explaining the diffuse scattering signal from protein crystals that arise from correlated protein motions (*Nature Comm* 2020, *Nature Comm* 2023). Many of the systems we study are metalloenzymes as they perform reactions of evolutionary significance, and we are highly experienced in anaerobic methods (*PNAS* 2017, *JBC* 2021, *PNAS* 2023). As a recognized expert in the structural biology community, I have served as an elected member of the U.S. National Committee for Crystallography (USNC/Cr) and am currently serving on the leadership for MacCHESS at the Cornell Energy High Synchrotron Source (CHESS) as well as the Northeastern Collaborative Access Team (NE-CAT) at the Advanced Photon Source (APS).

As a faculty member, I have taken on various roles in service to the scientific community. Of these, my most important work has been focused on two areas. As a leader in the X-ray community, I have actively worked to promote the advancement and education of X-ray science and structural biology. As a program chair for the 2020 American Crystallographic Association (ACA) Meeting, I was able to develop a program with a strongly educational theme, geared towards students and postdocs. In 2023, I directed the Erice International School of Crystallography, which drew ~70 students internationally. At every stage of my career, I have also worked to promote the advancement of women and underrepresented groups in STEM. At Princeton, I served in various capacities to assess departmental climate, improve the experience of women faculty, and create an REU program to increase diversity in STEM. Currently, at Cornell Chemistry, I am the co-chair of the diversity, equity, and inclusion (DEI) committee, the faculty advisor for Cornell Chemists for Outreach and Graduate Inclusion (COrGI), and the Director of Graduate Studies.

B. Positions, Scientific Appointments, and Honors

Positions and Employment

2001 Visiting Scholar, Center for Materials Science and Engineering, MIT, Cambridge, MA
2001-2008 Graduate Research Assistant, Department of Physics, Cornell University, Ithaca, NY
with Sol M. Gruner (Dept. of Physics and Cornell High Energy Synchrotron Source)
2008-2010 HHMI Postdoctoral Associate, Department of Chemistry, MIT, Cambridge, MA
with Catherine L. Drennan (HHMI, Depts. of Chemistry and Biology)
2010-2014 NIH Postdoctoral Fellow, Department of Chemistry, MIT, Cambridge, MA
with Catherine L. Drennan (HHMI, Depts. of Chemistry and Biology)
2014-2018 Assistant Professor of Chemistry, Princeton University, Princeton, NJ
2018-2021 Assistant Professor of Chemistry & Chemical Biology, Cornell University, Ithaca, NY
2019-present Graduate Faculty, Field of Biophysics, Cornell University, Ithaca, NY
2021-present Associate Professor of Chemistry & Chemical Biology, Cornell University, Ithaca, NY
2022-present Graduate Faculty, Field of Physics, Cornell University, Ithaca, NY
2024-present Faculty Fellow, Atkinson Center for Sustainability, Cornell University, Ithaca, NY
2024-present Director of Graduate Studies, Chemistry & Chemical Biology, Cornell University, Ithaca, NY

Other Experience and Professional Memberships

2006- Member, Biophysical Society
2007 Mentor, Cornell University Expand Your Horizon Program
2008- Reviewer for *Science, Nature, Nature Comm, JACS, Biochemistry, IUCr, Biophysical Journal, J Phys Chem, Langmuir, Nat Prod Rev, J Mol Biol, Chemical Science.*
2008 Training in the teaching of writing at the Cornell University Knight Institute
2009 HHMI MIT Mentoring Program in Chemical Biology
2010-2013 Member, American Physical Society
2010- Member, American Chemical Society
2011- Member, Protein Society
2011-2013 Elected Member, Cornell High Energy Synchrotron Source Executive User Committee
2014-2018 Proposal Reviewer, Cornell High Energy Synchrotron Source
2016 Organizer, *"Biomolecules in Motion"* Workshop, Cornell High Energy Synchrotron Source.
2016 Session chair, 2016 Diffraction Methods Gordon Research Conference
2016 Session chair, 21st Association for Crystallization Technology Larson Workshop
2017 Session chair, 2017 American Crystallographic Association Meeting
2017 Organizer, *"Measurement and Interpretation of Diffuse Scattering in X-Ray Diffraction for Macromolecular Crystallography"* Workshop, NSLS-II and CFN Meeting
2018 Session chair, 2018 Metallocofactors Gordon Conference
2019-present Member, Structural Biology Oversight Committee, Cornell Cryo-EM Facility
2019-present Faculty mentor, Chemical Biology Interface (CBI) Training Program, Cornell University
2019-2021 Elected member, U.S. National Committee for Crystallography (USNC/Cr)
2022-2023 Invited editor, *Methods in Enzymology*

Honors

2007 Best Instrumentation Poster Award, Cornell High Energy Synchrotron Source Users Meeting
2010 National Institutes of Health Ruth L. Kirschstein National Research Service Award (GM090486)
2012 Plenary speaker for 15th International Small Angle Scattering Conference, Sydney
2012 National Institutes of Health Pathway to Independence Award (GM100008)
2017 Invited Author, *Holy Grails in Chemistry* Special Issue of *Acc Chem Res*
2017 Invited Author, *Chemical Reviews*
2017 *Future of Biophysics* Burroughs Wellcome Fund Symposium Lecture, Biophysical Society.
2017 National Institutes of Health Maximizing Investigators' Research Award
2018 Invited Author, *Future of Biochemistry* Special Issue of *Biochemistry*
2020-2021 Program Chair, American Crystallographic Association Meeting
2020 Margaret C. Etter Early Career Award, American Crystallographic Association
2020 National Science Foundation CAREER Award
2020 *Future of Biophysics* Burroughs Wellcome Symposium Lecture, Biophysical Society

2022 Director, Erice International School of Crystallography
2022 Young Investigator Award, The Protein Society
2023 Editor, Methods in Enzymology
2024 Mildren Cohn Young Investigator Award, American Society for Biochem. & Molecular Biology

C. Contributions to Science

1) **Diffuse scattering from correlated motions in protein crystals**: Conventional crystallography involves analyzing sharp diffraction patterns, commonly called Bragg data. However, real crystals are not perfectly periodic and produce additional scattering between the Bragg peaks. This smooth background pattern, known as diffuse scattering, contains information about correlated displacements within the crystal but has been exceeding difficult to measure and interpret. My group is leading the world in the interpretation of macromolecular diffuse scattering, and we are making our software publicly available.
    a. Meisburger SP, Case DA, **Ando N**. (2023) "Robust total X-ray scattering workflow to study correlated motion of proteins in crystals." *Nature Communications* 14, 1228. PMCID: PMC9984388
    b. Meisburger SP, Case DA, **Ando N**. (2020) "Diffuse X-ray scattering from correlated motions in a protein crystal." *Nature Communications* 11, 1271. PMCID: PMC7062842
    c. Meisburger SP, Thomas WC, Watkins MB, **Ando N**. (2017) "X-ray scattering studies of protein structural dynamics." *Chem Rev* **117,** 7615–7672. PMCID: PMC5562295
    d. **Ando N**. Protein Folding & Dynamics Webinar (2021) – recording available online

2) **Evolution of allostery**: Ribonucleotide reductases (RNRs) are essential enzymes for all DNA-based life and have a fascinating evolutionary history that is thought to pre-date the oxygenation of the Earth. Among the RNR family the class Ib RNRs are unusual for two reasons: it lacks a regulatory domain that is prevalent in the rest of the RNR family, and it is found only in bacteria, including a number of well-known human pathogens. Using SAXS, crystallography, and cryo-EM, we discovered that a stunning form of convergent allostery had evolved in this class. Based on this discovery, we conducted a formal investigation of RNR evolution using phylogenetic inference, machine-learning methods, SAXS, and cryo-EM.
    a. Burnim AA, Xu D, Spence MA, Jackson CJ, **Ando N**. (2022) "Analysis of insertions and extensions in the functional evolution of the ribonucleotide reductase family." *Protein Sci*., 31:e4483.
    b. Burnim AA, Spence MA, Xu D, Jackson CJ*, **Ando N***. (2022) "Comprehensive phylogenetic analysis of the ribonucleotide reductase family reveals an ancestral clade and the role of insertions and extensions in diversification." *eLife*, 11: e79790. *co-corresponding.
    c. Thomas WC, Brooks PF, Burnim AA, Bacik J-P, Stubbe J, Kaelber JT, Chen JZ, **Ando N**. (2019) "Convergent allostery in ribonucleotide reductase." *bioRxiv* 504290 doi:10.1101/504290. *Nature Communications* 10, Article number: 2653. PMCID: PMC6572854
    d. **Ando N.** American Crystallographic Association (ACA) Etter Award Talk (2020) – recording available online

3) **Complex metalloenzymes**: My group is interested in understanding how life evolves and adapts to unusual environments. We have used various techniques to study metalloenzymes that perform challenging reactions with biomedical and evolutionary significance.
    a. Watkins MB, Wang H, Burnim AA, **Ando N**. "Conformational switching and flexibility in methionine synthase studied by small-angle X-ray scattering and cryo-electron microscopy." (2023) *PNAS* 120, e2302531120. PMCID: PMC10293825
    b. Illava G, Gillilan RE, **Ando N**. "Development of in-line anoxic small-angle X-ray scattering and structural characterization of an oxygen-sensing transcriptional regulator." (2023) J. Biol. Chem. 299: 105039. PMCID: PMC10425943
    c. Parker MJ, Maggiolo AO, Thomas WC, Kim A, Meisburger SP, **Ando N***, Boal AK*, and Stubbe J*. (2018) "An endogenous dAMP ligand in *Bacillus subtilis* class Ib RNR promotes assembly of a noncanonical dimer for regulation by dATP." *PNAS* **55,** 201800356–10. *co-corresponding. PMCID: PMC5960316
    d. Davis KM, Schramma K, Hansen W, Bacik J-P, Khare S, Seyedsayamdost M, **Ando N.** (2017) Structures of the peptide-modifying radical SAM enzyme SuiB elucidate the basis of substrate recognition. *PNAS* **114,** 10420–10425. PMCID: PMC5625900

4) **Service to the structural biology community:** I have a long track record of service to the field of structural biology. In addition to software contributions, a high-pressure small-angle X-ray scattering (SAXS) cell that I designed in my graduate studies has formed the basis for the recently established high-pressure biology (HP-Bio) beamline at the Cornell High Energy Synchrotron Source (CHESS). Notably, we have developed software for deconvolution of SAXS data, such as evolving factor analysis (EFA) and regularized alternating least-squares (REGALS). These and software packages for diffuse scattering data processing are available on our lab GitHub.
    a. Skou S, Gillilan RE, **Ando N.** (2014) "Synchrotron-based small-angle X-ray scattering (SAXS) of biomacromolecules in solution." *Nature Protocols* **9**, 1727–1739. PMCID: PMC4472361
    b. Meisburger SP, Taylor AB, Khan CA, Zhang S, Fitzpatrick PF, **Ando, N**. (2016) "Domain movements upon activation of phenylalanine hydroxylase characterized by crystallography and chromatography-coupled small-angle X-ray scattering." *JACS* **138,** 6506–6516. PMCID: PMC4896396
    c. Meisburger SP, Xu D, **Ando N**. (2021) "*REGALS*: a general method to deconvolve X-ray scattering data from evolving mixtures." *IUCrJ*, 8, 225-23.
    d. Ando Lab GitHub

5) **Allostery in a radical enzyme:** My postdoctoral work on class Ia ribonucleotide reductases (RNRs) set a new precedent for the use of SAXS to study transient and heterogeneous protein complexes. By combining SAXS with other biophysical techniques, we achieved a major milestone in understanding allosteric regulation of the class Ia RNR from *E. coli* and addressed a 50-year old mystery surrounding this complex system. This work has been included in the 6th edition of Lehninger, "Principles of Biochemistry."
    a. **Ando N**, Brignole EJ, Zimanyi CM, Funk MA, Yokoyama K, Asturias FJ, Stubbe J, Drennan CL. (2011) "Structural interconversions modulate activity of *Escherichia coli* ribonucleotide reductase." *PNAS* 108, 21046–21051. PMCID: PMC3248520
    b. Zimanyi CM, **Ando N**, Brignole EJ, Asturias FJ, Stubbe J, Drennan CL. (2012) "Tangled up in knots: Structures of inactivated forms of *E. coli* class Ia ribonucleotide reductase. "*Structure* 20, 1374–1383. PMCID: PMC3459064
    c. Minnihan EC, **Ando N**, Brignole EJ, Olshansky L, Chittuluru J, Asturias FJ, Drennan CL, Nocera D, Stubbe J. (2013) "Generation of a stable, aminotyrosyl radical-induced α2β2 complex of *Escherichia coli* class Ia ribonucleotide reductase." *PNAS* 110, 3835–3840. PMCID: PMC3593893
    d. **Ando N*,** Li H, Brignole EJ, Thompson S, McLaughlin MI, Page JE, Asturias FJ, Stubbe J, Drennan CL. "Allosteric inhibition of human ribonucleotide reductase by dATP entails the stabilization of a hexamer." 55, 373–381 (2016). *co-corresponding. PMCID: PMC4722859

Complete List of Published Work in Google Scholar:
https://scholar.google.com/citations?user=v-MyIFAAAAAJ&hl=en

BIOGRAPHICAL SKETCH

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NAME: Xiaokun Pei

eRA COMMONS USER NAME (credential, e.g., agency login): XIAOKUN_PEI

POSITION TITLE: Postdoctoral Associate

EDUCATION/TRAINING *(Begin with baccalaureate or other initial professional education, such as nursing, include postdoctoral training and residency training if applicable. Add/delete rows as necessary.)*

INSTITUTION AND LOCATION	DEGREE *(if applicable)*	Completion Date MM/YYYY	FIELD OF STUDY
Beijing Institute of Technology	B.Sc.	06/2016	Chemistry
University of California, Berkeley	Ph.D.	12/2021	Chemistry
Cornell University	Postdoc	Current	Chemistry

A. Personal Statement

I am a structural biology researcher from a synthetic chemistry background. My PhD research mainly focused on the syntheses and X-ray crystallography of a class of protein-like inorganic-organic hybrid material rich in disorder and structure dynamics. The first project during my Ph.D. study was to use a porous crystal to incorporate structure-unknown guest molecules and determine their crystal structures, during which my skills in chemical crystallography were rigorously trained. After that, I took on a collaborative project to study the disorder and structure dynamics of a material named ZIF-90. I conducted finely controlled data collection to obtain high-quality data that enabled precise interpretation of the Bragg information, and furthermore, I was introduced to diffuse scattering analysis and had a touch on its power beyond average structure.

I was attracted to biological research by dynamics in crystals. Currently in Ando lab, I continue this interest by learning diffuse scattering analysis on protein crystals for understanding protein dynamics. In addition, I work on a small class of ribonucleotide reductases (class Ø RNRs) hypothesized to be living fossils of RNRs' early evolutionary divergence. I used bioinformatics approach to locate the enzymes of interest to work on, while diving into structure characterizations with a combined approach by small-angle X-ray scattering, cryogenic electron microscopy, and X-ray crystallography.

B. Positions, Scientific Appointments, and Honors

2022 – Served as reviewers for *J. Am. Chem. Soc.*, *Microporous Mesoporous Mater.*, and *Crystals*.
2014 Excellent Student of Beijing (41 among approx. 20000 students), Beijing Education Committee
2013, 2014 National Scholarship (Top 1%), Ministry of Education of P. R. China

C. Contributions to Science

(1) Structural Biology on Enzyme Dynamics

a. **Pei, X.**;† Bhatt, N.;† Wang, H.; Ando, N,; Meisburger, S. Introduction to diffuse scattering and data collection. *Methods in Enzymology*, **2023**, *688*:1-42. (†co-first author)
b. Byer, A. S.; **Pei, X.**;† Patterson, M. G.;† Ando, N. Small-angle X-ray scattering studies of enzymes. *Curr. Opin. Chem. Biol.* **2023**, *72*, 102232. (†co-second author)

(2) Structures and Dynamics of Metal-Organic Frameworks

I have deep-dived into crystallographic characterization on chiral metal-organic frameworks (MOFs) developed from aluminum ion and various organic linkers. Aluminums – exist as metal-oxo clusters in these MOFs – greatly diversify the form of chirality of these MOFs beyond single-molecule level. Crystallography with topological analysis helped to reveal this complexity, forming a methodology to understand the chirality of extended systems. Furthermore, I expanded the scope of the host-guest chemistry of one of these MOFs, MOF-520, further analyzed the symmetry relations and disorder behaviors complexed by the covalently-attached guest molecules.

a. **Pei, X.**; Bürgi, H.-B.; Kapustin, E. A.; Liu, Y.; Yaghi, O. M. Coordinative Alignment in the Pores of MOFs for the Structural Determination of N-, S-, and P-Containing Organic Compounds Including Complex Chiral Molecules. *J. Am. Chem. Soc.* **2019**, *141*, 18862–18869.
b. Wang, H.;† **Pei, X.**;† Proserpio, D. M.; Yaghi, O. M. Design MOFs with Absolute Structures: A Case Study. *Israel. J. Chem.* **2021**, *61*, 1–9. (†co-first author)

MOFs are rich in dynamics, and I have been constantly seeking to capture them *in crystallo*. I and my collaborator came up with a strategy using variable temperature experiments to realize controlled release of the guest inside a MOF, thus allowing a movie-like observation of a water cycling dynamics within MOF-303 that has been long interested.

c. Hanikel, N.; **Pei, X.**; Chheda, S.; Lyu, H.; Jeong, W.; Sauer, J.; Gagliardi, L.; Yaghi, O. M. Evolution of Water Structures in Metal–Organic Frameworks for Improved Atmospheric Water Harvesting. *Science* **2021**, *374*, 454–459.

I have participated in multiple projects for crystallographic characterizations of MOFs under applications such as catalysis or battery, many of required special sample handling or advanced crystallographic techniques/procedures.

d. Lyu, H.; Chen, O. I.-F.; Hanikel, N.; Hossain, M. I.; Flaig, R. W.; **Pei, X.**; Amin, A.; Doherty, M. D.; Impastato, R. K.; Glover, T G.; Moore, D. R.; Yaghi, O. M. Carbon Dioxide Capture Chemistry of Amino Acid Functionalized Metal–Organic Frameworks in Humid Flue Gas. *J. Am. Chem. Soc.* **2022**, *144*, 2387–2396.
e. Lee, J. S.; Kapustin, E. A.; **Pei, X.**; Llopis, S.; Yaghi, O. M.; Toste, D. F. Architectural Stabilization of a Gold(III) Catalyst in Metal-Organic Frameworks. *Chem* **2020**, *6*, 142–152.
f. Xu, W.; **Pei, X.**; Diercks, C. S.; Lyu, H.; Ji, Z.; Yaghi, O. M. A Metal–Organic Framework of Organic Vertices and Polyoxometalate Linkers as a Solid-State Electrolyte. *J. Am. Chem. Soc.* **2019**, *141*, 17522–17526.
g. Matheu, R.; Gutierrez-Puebla, E.; Monge, Á. M.; Diercks, C. S.; Kang, J.; Prévot, M. S.; **Pei, X.**; Hanikel, N.; Zhang, B.; Yang, P.; Yaghi, O. M. Three-Dimensional Phthalocyanine Metal-Catecholates for High Electrochemical Carbon Dioxide Reduction. *J. Am. Chem. Soc.* **2019**, *141*, 17081–17085.
h. Abdel-Mageed, A. M.; Rungtaweevoranit, B.; Parlinska-Wojtan, M.; **Pei, X.**; Yaghi, O. M.; Behm, J. R. Highly Active and Stable Single-Atom Cu Catalysts Supported by a Metal–Organic Framework. *J. Am. Chem. Soc.* **2019**, *141*, 5201–5210. DOI:
i. Gao, X.; **Pei, X.**; Gardner, D. W.; Diercks, C. S.; Lee, S.; Rungtaweevoranit, B.; Prevot, M. S.; Zhu, C.; Fakra, S.; Maboudian, R. Casting Nanoporous Platinum in Metal–Organic Frameworks. *Adv. Mater.* **2019**, *31*, e1807553.
j. Baek, J.; Rungtaweevoranit, B.; **Pei, X.**; Park, M.; Fakra, S. C.; Liu, Y.-S.; Matheu, R.; Alshmimri, S. A.; Alshihri, S.; Trickett, C. A.; Somorjai, G. A.; Yaghi, O. M. Bioinspired Metal–Organic Framework Catalysts for Selective Methane Oxidation to Methanol. *J. Am. Chem. Soc.* **2018**, *140*, 18208–18216.
k. Ji, Z.; Trickett, C.; **Pei, X.**; Yaghi, O. M. Linking Molybdenum–Sulfur Clusters for Electrocatalytic Hydrogen Evolution. *J. Am. Chem. Soc.* **2018**, *140*, 13618–13622.