

# Curriculum vitae of Dorothee Liebschner, PhD

## Personal information

---

Name **Liebschner**  
First Name **Dorothee Claudia**  
Present affiliation Project Scientist, Molecular Biophysics and Integrated Bioimaging Division,  
Lawrence Berkeley National Laboratory, 1 Cyclotron Rd, Berkeley, CA  
94720, USA  
E-mail dcliebschner@lbl.gov

## Chronology of employment

---

12/2015 - present Lawrence Berkeley National Laboratory, Berkeley, USA  
*Position:* Project Scientist in Macromolecular Crystallography (MX)  
*Project:* Methods development; software development for MX data

09/2013 – 12/2015 Structural Biology Research Center, Photon Factory KEK, Tsukuba, Japan  
*Position:* Postdoctoral Researcher in MX  
*Project:* Sulphur SAD phasing at low X-ray energy

10/2011 – 08/2013 Macromolecular Crystallography Laboratory, National Cancer Institute,  
CCR/Argonne National Laboratory, Argonne, IL, USA  
*Position:* Postdoctoral Researcher in MX  
*Project:* Refinement of high resolution structures (PriB, Trypsin);  
Radiation damage; Accuracy of diffraction data

09/2007 – 07/2011 Laboratory Cristallographie, Résonance Magnétique et  
Modélisations (CRM2), Nancy, France  
*Position:* PhD student, “Allocataire de recherche”<sup>1</sup>  
*Project:* Electrostatic and structural properties of proteins diffracting  
at high resolution (PhD thesis)

---

<sup>1</sup> “Allocataire de recherche” is a PhD candidate who has obtained, based on their academic accomplishments, a 3-years position and is awarded a research grant. The selection is competitive and based on the ranking after the final exams in the first semester of the final Master academic year.

## Education:

---

Period	Name of the diploma	University
09/2007-11/2010	Doctoral degree in physics	University Henri Poincaré (UHP), Nancy, France
09/2006-08/2007	Master 2/ Diplomarbeit <sup>2</sup>	University Henri Poincaré (UHP), Nancy, France
09/2005-08/2006	Master 1	University Henri Poincaré (UHP), Nancy, France
09/2004-08/2005	Licence (Bachelor)	Saarland University (UdS), Saarbrücken, Germany
09/2003-08/2004	Vordiplom/DEUG/DPC U	Luxembourg University, Luxembourg
10/2002-08/2003	1st year physics	Saarland University (UdS), Saarbrücken, Germany
2002	Abitur <sup>3</sup> /baccalauréat (matriculation)	Robert-Schuman Secondary School, Saarlouis, Germany

## Full list of Publications

---

- 1) **Liebschner, D.** et al., Macromolecular structure determination using X-rays, neutrons and electrons: recent developments in Phenix, *Acta Cryst. D*, 75, 861-877 (2019). (doi: 10.1107/S2059798319011471)
- 2) Adams, P.D. *et al*, Announcing mandatory submission of PDBx/mmCIF format files for crystallographic depositions to the Protein Data Bank (PDB), *Acta Cryst. D*, 75, 451-545 (2019). (doi: 10.1107/S2059798319004522)
- 3) **Liebschner, D.**, Afonine, P. V., Moriarty, N. W., Langan, P. and Adams, P. D., Evaluation of models determined by neutron diffraction and proposed improvements to their validation and deposition, *Acta Crystallogr. Sect. D Biol. Crystallogr.* 74, 800-813 (2018).
- 4) **Liebschner, D.**, Book review: Protein Crystallography – Methods and Protocols. Edited by A. Wlodawer, Z. Dauter and M. Jaskolski. Humana Press, 2017. Pp XIII + 672. Hardcover. Price GBP 100, USD 159. ISBN 9781493969982. *Acta Cryst. F*, 74, 74-75 (2018), doi: 10.1107/S2053230X17017757
- 5) Moriarty, N. W., **Liebschner, D.**, Klei, H. E., Echols, N., Afonine, P. V., Headd, J. J., Poon, B. K. and Adams, P. D., Interactive Comparison and Remediation of Collections of Macromolecular Structures, *Protein Science*, 27, 182-194 (2018), doi: 10.1002/pro.3296

---

<sup>2</sup> Integrated study course in physics: studies in 3 different countries (Germany, Luxemburg and France), with a triple diploma after the second year and a double diploma after the 5th year (corresponds to Master2).

<sup>3</sup> The Abibac course yields the German and French diploma of secondary school (Abitur, baccalauréat) which qualifies for university admission or matriculation. Lectures and final exams in History and Geography are in French.

- 6) Nagae, M., **Liebschner, D.** et al. Crystallographic analysis of murine p24y2 Golgi dynamics domain. *Proteins Struct. Funct. Bioinforma.* 85, 764–770 (2017). (doi: 10.1002/prot.25242)
- 7) Sato, M., **Liebschner, D.** et al. The First Crystal Structure of a Family 129 Glycoside Hydrolase from a Probiotic Bacterium Reveals Critical Residues and Metal Co-factors. *J. Biol. Chem.* jbc.M117.777391 (2017). (doi: 10.1074/jbc.M117.777391)
- 8) Young, I. D. et al. Structure of photosystem II and substrate binding at room temperature. *Nature* 1–22 (2016). doi:10.1038/nature20161
- 9) **Liebschner, D.** et al. Polder maps: Improving OMIT maps by excluding bulk-solvent. *Acta Crystallogr. Sect. D Biol. Crystallogr.* 73, 148–157 (2017). (doi: [10.1107/S2059798316018210](https://doi.org/10.1107/S2059798316018210))
- 10) **Liebschner, D.**, Yamada, Y., Matsugaki, N., Senda, M. & Senda, T. On the influence of crystal size and wavelength on native SAD phasing. *Acta Crystallogr. Sect. D Struct. Biol.* 72, 728–741 (2016).
- 11) **Liebschner, D.**, Rosenbaum, G., Dauter, M. & Dauter, Z. Radiation decay of thaumatin crystals at three X-ray energies. *Acta Crystallogr. Sect. D Biol. Crystallogr.* 71, 772–778 (2015).
- 12) Elias, M.; **Liebschner, D.**; Koepke, J.; Lecomte, C.; Guillot, B.; Jelsch, C.; Chabriere, E., Hydrogen atoms in protein structures: High-resolution X-ray diffraction structure of DFPase, *BMC Research Notes* 2013, 6:308
- 13) **Liebschner, D.**; Dauter, M.; Brzuszkiewicz, A. & Dauter, Z., On the reproducibility of protein crystal structures: five atomic resolution structures of trypsin, *Acta Crystallographica Section D*, 2013, 69, 1447-1462
- 14) **Liebschner, D.**; Brzezinski, K.; Dauter, M.; Dauter, Z.; Nowak, M.; Kur, J. & Olszewski, M., Dimeric structure of the N-terminal domain of PriB protein from *Thermoanaerobacter tengcongensis* solved ab initio, *Acta Crystallographica Section D*, 2012, 68, 1680-1689
- 15) **Liebschner, D.**; Dauter, M.; Rosenbaum, G. & Dauter, Z., How good can our beamlines be?, *Acta Crystallographica Section D*, 2012, 68, 1430-1436
- 16) Domagala, S.; Fournier, B.; **Liebschner, D.**; Guillot, B. & Jelsch, C., An improved experimental databank of transferable multipolar atom models -- ELMAM2. Construction details and applications, *Acta Crystallographica Section A*, 2012, 68, 337-351
- 17) Jelsch, C.; Domagala, S.; Guillot, B.; **Liebschner, D.**; Fournier, B.; Pichon-Pesme, V. & Lecomte, C., Gatti, C. & Macchi, P. (Eds.), Frontier Applications of Experimental Charge Density and Electrostatics to Bio-macromolecules, *Modern Charge-Density Analysis*, Springer, 2012, 527-552
- 18) Elias, M.; **Liebschner, D.**; Gotthard, G. & Chabriere, E., Structural insights and ab initio sequencing within the DING proteins family, *Journal of Synchrotron Radiation*, 2011, 18, 45-49

- 19) **Liebschner, D.**; Jelsch, C.; Espinosa, E.; Lecomte, C.; Chabrière, E. & Guillot, B., Topological Analysis of Hydrogen Bonds and Weak Interactions in Protein Helices via Transferred Experimental Charge Density Parameters, invited paper in special issue in honor of R. Bader *The Journal of Physical Chemistry A*, **2011**, *115*, 12895-12904
- 20) **Liebschner, D.**; Elias, M.; Moniot, S.; Fournier, B.; Scott, K.; Jelsch, C.; Guillot, B.; Lecomte, C. & Chabrière, E., Elucidation of the Phosphate Binding Mode of DING Proteins Revealed by Subangstrom X-ray Crystallography, *JACS*, **2009**, *131*, 7879-7886
- 21) Krüger, J. K.; Müller, U.; Bactavatchalou, R.; **Liebschner, D.**; Sander, M.; Possart, W.; Wehlack, C.; Baller, J. & Rouxel, D., Mechanical Interphases in Epoxies as seen by Nondestructive High-Performance Brillouin Microscopy, *Adhesion, Wiley*, **2006**, 125-142

## Conferences/Workshops

---

October 19-30, 2019, Cold Spring Harbor Course X-Ray Methods in Structural Biology, Cold Spring Harbor Laboratory, NY (US). Role: Assistant. **Lecture:** Maps: from Fo-Fc to 2mFo-Fc, omit and Polder maps.

October 8-10, 2019, Instruct Workshop on Integration of Computational Approaches in Structural Biology, Vestec, Czech Republic, **Invited talk:** CryoEM model building and other tools in Phenix

September 22-27, Phenix Workshop, Duke, NC (US), **Oral presentation:** 1) nonbonded overlaps, 2) neutron models

August 18-23, European Crystallographic Meeting, Vienna (Austria), **Invited Talk** (MS02-02): Polder Maps: Improving OMIT Maps for Ligand Building and Validation; **Teaching presentation:** satellite workshop "Low resolution structure determination and refinement of biological macromolecules by crystallography and cryo-EM", August 18

August 14-17, European Crystallographic Computing Forum, Melk (Austria), **Teaching presentation:** CCTBX tutorial

June 17-24, 2018, CCP4/APS School in Macromolecular Crystallography: From data collection to structure refinement and beyond, **Teaching presentation:** Phasing and automation in Phenix

May 5-10, 2019, Rapidata, SLAC National Laboratory, Stanford (US), **Teaching presentation:** Solve and Phenix

West Coast Structural Biology Workshop, Asilomar, CA (US), March 17-20, 2019, **Poster presentation:** cryoEM re-refine

March 11-14, 2019, Phenix Workshop, Berkeley, CA (USA). **Oral presentation:** Phenix article

Bay Area Cryo-EM meeting, November 29, 2018, Genentech, South San Francisco, CA (US). **Poster presentation:** cryoEM re-refine

September 17-20, 2018, Phenix Workshop, Cambridge (UK). **Oral presentation:** 1) cryo-EM RErefine 2) updates on the tutorial channel.

August 2-7 , 2018, Gordon Research Conference Diffraction Methods in Structural Biology, Bates College, Lewiston, ME (US). **Invited talk:** Polder maps - Improving OMIT maps by accounting for bulk solvent.

July 19-25, 2018, ACA (American Crystallographic Association) meeting, Toronto (Canada). **Invited talk:** Polder maps - Improving OMIT maps for ligand building and validation.

June 18-25, 2018, CCP4/APS School in Macromolecular Crystallography: From data collection to structure refinement and beyond, **Teaching presentation:** Phasing and automation in Phenix

April 22-27, 2018, Rapidata, SLAC National Laboratory, Stanford (US), **Teaching presentation:** Phenix tutorials

March 26-29, 2018, Phenix Workshop, Santa Fe, NM (USA). **Oral presentation:** 1) validation of H atoms 2) Weekly re-refinements.

September 24-29, 2017, Phenix Workshop, Duke, NC (USA). **Oral presentation,** title: "1) Riding hydrogen atoms 2) Updates on the tutorial channel"

August 21-28, 2017, 24<sup>th</sup> IUCr conference, Hyderabad (India). **Oral presentation:** MS-001, title: Polder maps: Improving OMIT maps for ligand building and validation. **Session chair:** MS-028 Long wavelength applications in macromolecular crystallography. **Oral presentation:** Software Fayre, title: "Phenix". **Oral presentation:** Satellite Meeting "Phasing and Model Building", title: Visualizing ligands with Polder maps

May 13-17, 2017, Understanding Biology through Structure, Santa Fe, NM (USA), **Poster presentation:** Polder maps: Improving OMIT maps for ligand building and validation

West Coast Protein Crystallography Workshop, Asilomar, CA (US), March 19-22, 2017, **Poster presentation:** Polder maps: Improving OMIT maps for ligand building and validation

March 13-16, 2017, Phenix Workshop, Berkeley, CA (USA), **Oral presentation:** How to make a Phenix video tutorial?

September 12-15, 2016, Phenix Workshop, Cambridge (UK), **Oral presentation:** 1) Riding hydrogen atoms 2) Phenix video tutorial

March 14-17, 2016, Phenix Workshop, Santa Fe, NM (USA), **Oral presentation:** Polder maps: Improving OMIT maps for ligand building and validation

July 25-29, 2015, ACA (American Crystallographic Association) meeting, Philadelphia, PA (USA), **Oral presentation:** The challenges of soft X-rays: Data collection above 3 Å wavelength

June 24-26, 2015, 15<sup>th</sup> annual meeting of the Protein Science Society of Japan, Tokushima (Japan), **Poster presentation:** Softer but stronger? Sulfur SAD with low energy X-rays.

March 12, 2015, WINTech 2015 (Workshop on Innovation and Pioneering Technology), Kobe (Japan)

August 5-12, 2014, IUCr conference, Montreal (Canada), **Oral presentation:** Softer but stronger? Sulfur SAD with X-rays of 2.7 Å and 1.9 Å wavelength

April 10-12, 2014, Eighth International Workshop on X-ray Radiation Damage to Biological Crystalline Samples, EMBL Hamburg (Germany)

July 20-24, 2013, ACA (American crystallographic association) meeting, Honolulu, HI (USA), **Poster presentation:** Ten thousand shades of Gray: The Blake&Phillips radiation damage decay model revisited

June 24-28, 2013, 4th Workshop on Neutron Scattering Applications in Structural Biology, Oak Ridge, TN (USA). **Poster presentation:** Dimeric structure of the N-terminal domain of PriB protein from *Thermoanaerobacter tengcongensis*

June 2-7, 2013, Pushing the Limits of Experimental and Theoretical Charge and Spin Density Studies, Les Diablerets (Switzerland). **Invited talk:** On the reproducibility of protein crystal structures: five atomic resolution structures of trypsin

March 9-15, 2013, Synchrotron Charge Density School, Advanced Photon Source, Argonne, IL (USA)

August 6-11, 2012, 27<sup>th</sup> European Crystallographic Meeting, Bergen (Norway). **Invited talk:** Topological analysis of hydrogen-bonds and weak interactions in protein helices

July 15-20, 2012, Gordon Research Conference: Diffraction Methods in Structural Biology, Bates College, Lewiston, ME (USA). **Poster presentation:** Dimeric structure of the N-terminal domain of PriB protein from *Thermoanaerobacter tengcongensis*

May 31 - June 2 2012, 42<sup>nd</sup> Mid-Atlantic Macromolecular Crystallography Meeting, University of Virginia, Charlottesville, VA (USA)

March 14-16, 2012, Seventh International Workshop on X-ray Radiation Damage to Biological Crystalline Samples, Diamond Light Source (UK)

December 8-11, 2009, GT Bio, Paris (FR). **Oral presentation:** Elucidation of the phosphate binding mode of DING proteins (transl. from French)

October 28-30, 2009, International Workshop about the analysis of the electron density obtained by X-ray diffraction (transl. from French), Marrakech (Morocco)

July 6-12, 2009, Workshop in Biocrystallography (transl. from French), AFMB laboratory, Marseille (FR)

August 23-31, 2008, IUCr conference, Osaka (JP), **Poster presentation:** Protein helix-dipole calculations based on experimental electron densities

February 17 - March 20, 2008, HERCULES course, Grenoble (France). **Poster presentation:** Projects based on ultra high-resolution proteins

October 8-11, 2007, GT Bio Lille (FR), **Poster presentation:** ultra-high resolution refinement of DFPase (transl. from French)

2006, Workshop: Introduction to spatial physics, Liège (Belgium)

March 4-9, 2005, German physical society (DPG) conference, Berlin (GER)

---

## Teaching

---

### Selected presentations:

October 19-30, 2019, Cold Spring Harbor Course X-Ray Methods in Structural Biology, Cold Spring Harbor Laboratory, NY (US). Role: Assistant. **Lecture:** Maps: from Fo-Fc to 2mFo-Fc, omit and Polder maps.

August 14-17, European Crystallographic Computing Forum, Melk (Austria), **Lecture:** CCTBX tutorial

June 17-24, 2018, CCP4/APS School in Macromolecular Crystallography, **Lecture:** Phasing and automation in Phenix

May 5-10, 2019, Rapidata, SLAC National Laboratory, Stanford (US), **Lecture:** Solve and Phenix

June 18-25, 2018, CCP4/APS School in Macromolecular Crystallography, **Lecture:** Phasing and automation in Phenix

April 22-27, 2018, Rapidata, SLAC National Laboratory, Stanford (US), **Lecture:** Phenix tutorials

### Other:

Responsible for the *Phenix* tutorials YouTube channel ([www.youtube.com/c/phenixtutorials](http://www.youtube.com/c/phenixtutorials)), which features video tutorials on *Phenix* tools. The videos explain basic principles of each program, describe how to execute the tool and how to interpret the results. As of November 2019, the channel has more than 650 subscribers and 41k views.

## Language skills:

---

German	Native language
English	Fluent in writing, hearing and speaking
French	Fluent in writing, hearing and speaking (has French matriculation "baccalauréat")
Japanese	Basic knowledge in writing, hearing and speaking (passed the test JLPT <sup>4</sup> level 4 and 3)

---

<sup>4</sup> The JLPT (Japanese Language Proficiency Test) is a language test organised by the Japan Foundation. There are 5 different levels, level 1 being the most difficult.