Personal Information

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Citizenship India

Academic Appointments

Oct. 2019 - Present **Lawrence Berkeley National Laboratory**,
Research Scientist.

Aug. 2017 - Sep. 2019 **Lawrence Berkeley National Laboratory**,
Project Scientist.

Jan. 2017 - July 2017 **Lawrence Berkeley National Laboratory**,
Postdoctoral Research Associate.

July 2015 - Dec. 2016 **Center for Free-Electron Laser Science**, *Deutsches Elektronen-Synchrotron*,
Postdoctoral Research Associate.

July 2012 - June 2015 **University of Wisconsin-Milwaukee**, *Department of Physics*, USA,
Postdoctoral Research Associate.

May 2006 - Aug. 2006 **University of Southern California**, *Collaboratory for Advanced Computing And Simulations*, USA,
Visiting Scholar.

Education

May 2012 **Doctor of Philosophy in Physics**, *University of Wisconsin-Milwaukee*, USA, Department of Physics.

Dissertation First-principles studies of polar oxide surfaces and hetero-interfaces.

Supervisor Michael Weinert

May 2005 **Bachelor of Technology**, *Indian Institute of Technology, Kanpur*, India, Materials and Metallurgical Engineering.

Awards and Funding

June 2019 **Early Career Track LDRD**, *Lawrence Berkeley National Laboratory*.

May 2011 **The Papastamatiou Scholarship for outstanding performance in Theoretical Physics**, *Department of Physics*, University of Wisconsin-Milwaukee.

Publications

Building Mathematics, Algorithms, and Software for Experimental Facilities, *H. Chang, J. J. Donatelli, P. Enfedaque, G. Freychet, M. Haranczyk, et al.*, Handbook on Big Data and Machine Learning in the Physical Sciences, World Scientific Series on Emerging Technologies, 2020.

Ab initio structure determination from experimental fluctuation X-ray scattering data, *K. Pande, J. J. Donatelli, E. Malmerberg, L. Foucar, C. Bostedt, I. Schlichting, and P. H. Zwart*, PNAS, **115**, 2018.

Free-electron laser data for multiple-particle fluctuation scattering analysis, *K. Pande, J. J. Donatelli, E. Malmerberg, et al.*, Scientific Data, **5**, 2018.

Enzyme intermediates captured "on the fly" by mix-and-inject serial crystallography, *J. L. Olmos, S. Pandey, J. M. Martin-Garcia, et al.*, BMC Biology, **16**, 2018.

Continuous diffraction of molecules and disordered molecular crystals, *H. N. Chapman, O. M. Yefanov, K. Ayyer, T. A. White, A. Barty, A. Morgan, V. Mariani, D. Oberthuer, and K. Pande*, J. Appl. Cryst., **50**, 2017.

Mix-and-diffuse serial synchrotron crystallography, *K. R. Bayerlein, D. Dierksmeyer, V. Mariani, et al.*, IUCrJ, **4**, 2017.

Structural enzymology using X-ray free electron lasers, *C. Kupitz, J. L. Olmos, M. Holl, L. Tremblay, K. Pande, et al.*, Structural Dynamics, **4**, 2016.

The room temperature crystal structure of a bacterial phytochrome determined by serial femtosecond crystallography, *P. Edlund, H. Takala, E. Claesson, L. Henry, et al.*, Nature Scientific Reports, **6**, 2016.

Femtosecond structural dynamics drives trans/cis isomerization in photoactive yellow protein, *K. Pande, C. .D. M. Hutchinson, G. Groenhoff, A. Aquila, J. S. Robinson, J. Tenboer, S. Basu, S. Boutet, D. P. DePonte, et al.*, Science, **352**, 2016.

Room temperature structure beyond 1.5 Å by serial femtosecond crystallography, *M. Schmidt, K. Pande, S. Basu, and J. Tenboer*, Structural Dynamics, **2**, 2015.

Simulations on time-resolved structure determination of uncrystallized biomolecules in the presence of shot noise, *K. Pande, M. Schmidt, P. Schwander and D. K. Saldin*, Structural Dynamics, **2**, 2015.

Investigation of NO_2 adsorption on reduced graphene oxide, *E. C. Mattson, K. Pande, S. Cui, M. Weinert, J. H. Chen, and C. J. Hirschmugl*, Chem. Phys. Letters, **622**:86-91, 2015.

Time-resolved serial femtosecond crystallography captures high-resolution intermediates of photoactive yellow protein, *J. Tenboer, S. Basu, N. Zatsepin, K. Pande, D. Milathianski, M. Frank, M. Hunter, S. Boutet, G. Williams, J. E. Koglin, et al.*, Science, **346**:1242-1246, 2014.

Deducing fast electron density changes in randomly oriented uncrystallized biomolecules in a pump-probe experiment, *K. Pande, P. Schwander, M. Schmidt and D. K. Saldin*, Phil. Trans. R. Soc. B, **369**:20130332, 2014.

Vibrational excitations and low energy electronic structure of epoxide-decorated graphene, *E. C. Mattson, J. E. Johns, K. Pande, R. A. Bosch, S. Cui, M. Gajdardziska-Josifovska, M. Weinert, J. H. Chen, M. C. Hersham and C. J. Hirschmugl*, J. Phys. Chem. Lett, **5**:1, 2014.

Exploring adsorption and reactivity of NH_3 on reduced graphene oxide, *E. C. Mattson†, K. Pande†, M. Unger, S. Cui, G. Lu, M. Gajdardziska-Josifovska, M. Weinert, J. Chen, and C. J. Hirschmugl*, J. Phys. Chem. C, **117**:20, 2013.
† contributed equally

Atomic and electronic structure of polar Fe_2O_3(0001)/MgO(111) interfaces, *K. Pande, M. Gajdardziska-Josifovska, and M. Weinert*, Phys. Rev. B, **86**:035431, 2012.

Effects of unreconstructed and reconstructed polar surface terminations on growth, Structure, and magnetic properties of hematite films, *S. H. Cheung, A. Celik-Aktas, P. Dey, K. Pande, M. Weinert, B. Kabius, D. J. Keavney, S. A. Chambers and M. Gajdardziska-Josifovska*, Phys. Rev. B, **85**:045405, 2011.

Atomic and electronic structure of polar Fe_2O_3(0001)/MgO(111) interface, *K. Pande, M. Gajdardziska-Josifovska, and M. Weinert*, Microscopy and Microanalysis, **16**:657, 2010.

Past Teaching Experience

Teaching Assistantship, *University of Wisconsin-Milwaukee*, Department of Physics.

Fall '11 Grader and Tutor for Electrodynamics: A graduate course formally dealing with electrostatics and magnetostatics, Maxwell's equations, Faraday's law, and advanced mathematical techniques.

Fall '05, Spring '06 Laboratory for Physics in Everyday Life: A lab programmed to introduce non-science majors to the foundations of classical physics.

Invited Talks and Seminars

January 2020 **7^{th} BioXFEL International Conference**.
San Juan, PR

July 2019 **American Crystallographic Association**.
Covington, KY

April 2019 **BER Advisory Committee**.
Gaithersburg, MD

August 2017 **IUCr Congress**.
Hyderabad, India

July 2016 **Gordon Research Conference**.
Bates College, ME

March 2015 **Coherent Imaging Division Seminar**.
Center for Free-Electron Laser Science, Germany

February 2015 **Colloquium**.
Max-Planck Institute, Heidelberg, Germany

October 2014 **Biophysics Seminar**.
Dept. of Physics at University of Wisconsin, Milwaukee

April 2014 **NSF Advanced Postdoctoral Seminar Program for the UW System**.
Dept. of Physics at University of Wisconsin, Whitewater

Contributed Talks and Seminars

July 2018 **Gordon Research Conference**, *Bates College, ME.*

August 2016 **Meeting of the European Crystallographic Association**, *Basel, Switzerland.*

August 2015 **Meeting of the European Crystallographic Association**, *Rovinj, Croatia.*

August 2015 **Advanced Software Development Workshop**, *Rovinj, Croatia.*

February 2015 **2^{nd} Meeting on Structural Biology with FELs**, *Schloss Ringberg, Germany.*

January 2015 **2^{nd} International BioXFEL Conference**, *Ponce, Puerto Rico.*

October 2013 **1^{st} International BioXFEL Conference**, *London and Chicheley, UK.*

August 2010 **Microscopy and Microanalysis Meeting**, *Portland, Oregon, USA.*

June 2010 **70^{th} Physical Electronics Conference**, *University of Wisconsin-Milwaukee, WI, USA.*

March 2010 **March Meeting of the American Physical Society**, *Portland, Oregon, USA.*

June 2009 **69^{th} Physical Electronics Conference**, *Rutgers University, New Jersey, USA.*

March 2009 **March Meeting of the American Physical Society**, *Pittsburgh, Pennsylvania, USA.*

March 2008 **March Meeting of the American Physical Society**, *New Orleans, Louisiana, USA.*

Outreach

2018 **User Research Facilities, Washington DC**, *Volunteer.*

2016 **International Summer School of Crystallography, CFEL**, *Organiser.*

2015 **Wisconsin Science Olympiad**, *Volunteer.*

2014 **Wisconsin Science Olympiad**, *Volunteer.*

2006-08 **University of Wisconsin-Milwaukee Open House**, *Volunteer.*

Academic References

1 **Prof. James A. Sethian**,
Computational Research Division, Lawrence Berkeley National Laboratory
Email: jasethian@lbl.gov.

2 **Dr. Petrus H. Zwart**,
Molecular Biophysics and Integrated Bioimaging, Lawrence Berkeley National Laboratory
Email: phzwart@lbl.gov.

3 **Prof. Henry N. Chapman**,
Coherent Imaging Division, Center for Free-Electron Laser Science, Deutsches Elektronen-Synchrotron (DESY)
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4 **Prof. Marius Schmidt**,
Department of Physics, University of Wisconsin - Milwaukee
Email: smarius@uwm.edu.