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Institute of Physical Chemistry
Department of Theoretical Chemical Biology
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Education

Nagoya University

Degree: Doctor of Science, October 30, 2009

Advisors: Professor Takahisa Yamato

Nagoya University

Degree: M.S. Physics, May 31, 2007

Advisors: Professor Takahisa Yamato

Nagoya University

Degree: B.S. Physics, May 31, 2005

Advisors: Professor Takahisa Yamato

Professional Experience

April 2011

– Present

Postdoctoral Associate, Karlsruhe Institute of Technology

(Supervisor: Professor Marcus Elstner)

- The structural modeling of Channelrhodopsin
- Development of analyzing techniques on proteins

April 2009

– March 2011

JSPS Research fellow, Nagoya University

(Supervisor: Professor Takahisa Yamato)

- The color tuning mechanism of conger rhodopsin
- The structural disorder and inhomogeneous broadening of absorption spectrum of photoreceptor.

April 2007

– March 2009

Research Assistant, Nagoya University

(Supervisor: Professor Takahisa Yamato)

- Theoretical modeling of O-intermediate structure of bacteriorhodopsin.

April 2005

– March 2007

Researcher, Nagoya University

(Supervisor: Professor Takahisa Yamato)

- Theoretical study on the conformational change from the neutral form to the acid blue form of bacteriorhodopsin.

February 2005

– June 2009

Teaching Assistant, Nagoya University

(Supervisor: Takahisa Yamato)

- Taught classical mechanics and physical mathematics

Publications

– English

- (1) “QM/MM Simulations of Vibrational Spectral in Bacteriorhodopsin and Channelrhodopsin-2” K. Welke, H. C. Watanabe, T. Wolter, and M. Elstner *Phys. Chem. Chem. Phys.* (2013) **15**, 6651-6659
- (2) “Towards an understanding of channelrhodopsin function: Simulations lead to novel insights of channel mechanism” H. C. Watanabe, K. Welke, D. J. Sindhikara, P. Hegemann, and M. Elstner *J. Mol. Biol.* (2013) **425**, 1795-1814
- (3) “Rotamer Decomposition and Protein Dynamics – Efficiently Analyzing Dihedral Populations from Molecular Dynamics” H. Watanabe, M. Elstner, and T. Steinbrecher *J. Comp. Chem.* (2013) **34**, 3, 198-205
- (4) “Structural model of channelrhodopsin” H. C. Watanabe, K. Welke, F. Schneider, S. Tsunoda, F. Zhang, K. Deisseroth, P. Hegemann, and M. Elstner, *J. Biol. Chem.* (2012) **287**, 10, 7456-7466
- (5) “Color Tuning in Binding Pocket models of the Channelrhodopsin” K. Welke, J. Fraehmcke, H. C. Watanabe, P. Hegemann, and M. Elstner, *J. Phys. Chem. B* (2011) **115**, 15119-15128
- (6) “Molecular Mechanism of long-range synergetic color tuning between multiple amino acid residues in conger rhodopsin” H. C. Watanabe, Y. Mori, T. Tada, S. Yokoyama, and T. Yamato *Biophysics* (2010) **6**, 67-78
- (7) “The theoretical modeling of O-intermediate structure of bacteriorhodopsin” H. C. Watanabe, T. Ishikura, T. Yamato *Proteins*, (2009) **75**, 1, 53-61
- (8) “Spectral tuning of Photoactive yellow protein” T. Yamato, T. Ishikura, T. Kakitani, K. Kawaguchi, and H. Watanabe *Photochem. Photobiol.* (2007) **83**, 323-327

– Japanese

Prospects of FCS: Hiroshi Watanabe *Computation Center NEWS, Nagoya University* **6**, 4, 361-366

Selected Presentations

- Feb. 2013 **Poster:** “Towards an understanding of channelrhodopsin function: Simulations lead to novel insights of channel mechanism ”
Review meeting for the second funding period of DFG research Unit 1279
“Protein-based photoswitches as optogenetic tool”
- Oct. 2012 **Invited Talk:** “*Computational challenge in protein structural modeling*”
International Symposium on Computics: Quantum Simulation and Design
- Sep. 2012 **Poster:** “*Structural modeling of Channelrhodopsin*”
15th International Conference on Retinal Proteins
- Apr. 2012 **Talk:** “*Structural modeling of Channelrhodopsin*”
Computer simulation and theory of macromolecules 2012
- May 2012 **Talk:** “*Structural modeling of Channelrhodopsin*”
Annual meeting for 1279
- May 2011 **Talk:** “*Structural modeling of Channelrhodopsin*”
Annual meeting for 1279
- Apr. 2011 **Poster:** “*Structural modeling of Channelrhodopsin*”
Computer simulation and theory of macromolecules 2011
- May 2010 **Poster:** “*Structural analysis for Volvox Channel rhodopsin-1 based on homology model*”
The meeting of Channel rhodopsin and light-gated enzyme
- Jun. 2009 **Talk:** “*Spectral Tuning mechanism of Conger rhodopsin*”
The 36th Annual Meeting of Japan Society for Biomolecular Science
- Mar. 2009 **Talk&Poster:** “*On the spectral property of retinal proteins-inhomogeneity and static disorder*”
Biophysical Society of Chubu branch of Japan
- Dec. 2008 **Poster:** “*On the spectral property of retinal proteins-inhomogeneity and static disorder*”
The 46th Annual meeting of The Biophysical Society of Japan
- Nov. 2008 **Poster:** “*Theoretical modeling of the O-intermediate structure of bacteriorhodopsin*”
The 22nd Annual Meeting of The Molecular Simulation Society of Japan
- Jun. 2008 **Poster:** “*Theoretical modeling of the O-intermediate structure of bacteriorhodopsin*”
The 13th International Conference of Retinal Proteins.
- Jan. 2008 **Talk:** “*Theoretical modeling of the O-intermediate structure of bacteriorhodopsin*”
The 5th Open Workshop for “Chemistry of Biological Processes Created by Water and Biomolecules”
- Nov. 2007 **Talk:** “*Theoretical modeling of the O-intermediate structure of bacteriorhodopsin*”
Workshop on Computational Biophysics.
- Sep. 2007 **Talk:** “*Theoretical study of the acid blue form of bacteriorhodopsin*”
Annual Meeting of Japan Society for Molecular Science 2009
- Mar. 2007 **Talk:** “*Molecular Dynamics of Bacteriorhodopsin in acid blue form*” The Physical Society of Japan; 2007 Spring Meeting

Awards

Apr. 2010
– Mar. 2012

Excellent Young Researchers Overseas Visit Program

Apr. 2009
– Mar. 2011

Research Fellowship for Young Scientists, Japan Society for the Promotion of Science

Mar. 2009

Award for Young Scientists, Biophysical Society of Japan - Chubu -
For excellence in presentation.

Nov. 2008

Award for Student, the 22nd Annual Meeting of Molecular Simulation Society of Japan
For excellence in presentation

April 2007
– March 2009

Nagoya University Fellowship

Professional Memberships:

Biophysical Society of Japan