Yuko OKAMOTO

Position	Professor
Lab/Group	Theoretical Biophysics Laboratory (TB Lab)
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Education and Degrees

June, 1979, *B.S.-M.S.*, Brown University (Grew Foundation Scholar)

August, 1984, *Ph.D.*, Cornell University

Positions

September, 1984 – March, 1986, *Postdoctoral Research Associate*, Department of Physics, Virginia Polytechnic Institute and State University

April, 1986 – May, 1993, *Assistant Professor*, Department of Physics, Nara Women's University

May, 1993 – March, 1995, *Associate Professor*, Department of Physics, Nara Women's University

April, 1995 – March, 2005, *Associate Professor*, Department of Theoretical Studies, Institute for Molecular Science, Okazaki National Research Institutes (presently, National Institutes of Natural Sciences)

October, 1995 – March, 2005, *Associate Professor* (Joint Appointment), Department of Functional Molecular Science, The Graduate University for Advanced Studies

April, 2005 – present, *Professor*, Department of Physics, Graduate School of Science, Nagoya University

February, 2007 – present, *Professor* (Joint Appointment), Structural Biology Research Center, Graduate School of Science, Nagoya University

June, 2010 – present, *Professor* (Joint Appointment), Information Technology Center, Nagoya University

April, 2011 – present, *Professor* (Joint Appointment), Center for Computational Science, Graduate School of Engineering, Nagoya University

Honors

Fellow, American Physical Society (November 22, 2010)

nominated by: Division of Computational Physics (DCOMP)

citation: For his invention of novel and useful computational methodologies for probing the conformational phase space of biomolecules.

Overseas Visiting Scholar, St John's College, University of Cambridge (October – December, 2011: Michaelmas Term)

Research

Fields: biophysics, computational physics, computational chemistry

Keywords: computer simulation of biomolecular systems, generalized-ensemble algorithm, multicanonical algorithm, simulated tempering, replica-exchange method

There are a huge number of local-minimum-energy states in systems with many degrees of freedom such as biomolecular systems. Computer simulations of these systems tend to get trapped in these local-minimum states, giving wrong results. In order to overcome this difficulty, we introduced the generalized-ensemble algorithms to biomolecular simulations and have been developing new generalized-ensemble algorithms suitable for these systems. With these powerful simulation methods, we study the mechanisms of various biological phenomena. We have been studying the predictions of three-dimensional structures of proteins, protein folding problem, structural changes of proteins under high pressure, free energy calculations of docking of drug candidate molecules to proteins, formations of amyloid fibrils which are considered to be the cause of amyloid diseases, etc. Besides proteins, we also perform simulations of nucleic acids, lipid bilayers, oligosaccharide molecules, etc.

Nagoya University Faculty Profile Page (link)

Lab/Group Homepage (link)

List of Publications

Google Scholar (link)

ResearcherID (link)