

---

---

一般社団法人日本生物物理学会 第4回 Biophysics and Physicobiology  
論文賞受賞講演会

The 4<sup>th</sup> Award Seminar of Outstanding Biophysics and Physicobiology Paper

オーガナイザー：日本生物物理学会 Biophysics and Physicobiology 論文賞選考委員会

Organizers: Award committee for Outstanding Biophysics and Physicobiology Paper

日時：9月13日（日）12:50～13:20 / Sep. 13 Sun.

場所：H会場（大講義室A） / Room H (Lecture Room A)

形式：講演会 / Lecture

---

第4回 Biophysics and Physicobiology 論文賞受賞者

BPPB Outstanding Paper Awardee

林 智彦<sup>1</sup>, 松浦 東<sup>2</sup>, 佐藤 博之<sup>2</sup>, 櫻井 実<sup>3</sup>

Tomohiko Hayashi<sup>1</sup>, Azuma Matsuura<sup>2</sup>, Hiroyuki Sato<sup>2</sup>, Minoru Sakurai<sup>3</sup>

<sup>1</sup> 京都大学エネルギー理工学研究所 <sup>2</sup> 富士通研究所 <sup>3</sup> 東京工業大学バイオ研究基盤支援総合センター

<sup>1</sup> Institute of Advanced Energy, Kyoto University <sup>2</sup> Fujitsu Laboratories, Ltd. <sup>3</sup> Center for Biological Resources and Informatics, Tokyo Institute of Technology

全原子量子化学計算による光活性タンパク質の吸収波長制御機構の解析

Analyses of the spectral-tuning mechanisms of several photoactive proteins

based on the full-quantum chemical calculations

---

The photoactive proteins, which absorb light and convert it into biological signal or chemical energy, consist of a chromophore and an apoprotein. The absorption spectra of each protein are finely tuned due to the chromophore-apoprotein interactions. Elucidation of this spectral-tuning mechanism has been a central issue in biophysics. A typical theoretical approach toward achieving such elucidation is that the protein of interest is regarded as a hybrid system consisting of quantum-mechanical (QM) and molecular-mechanical (MM) regions (QM/MM). In this approach, the chromophore alone or a small region involving the chromophore and its neighboring amino acid residues are treated using a QM method, and its surrounding is approximated using a classical MM method. However, QM/MM approaches have some ambiguity concerning how to partition the system into QM and MM regions. To overcome this ambiguity, we developed a “Full-QM” theoretical approach and successfully applied it to the absorption-maximum calculations of several photoactive proteins. In our BIOPHYSICS paper in 2012[1], we analyzed the spectral-tuning mechanism of bacteriorhodopsin (bR), and showed that an important factor contributing to the spectral tuning of bR is the electron transfer from the apoprotein to the chromophore upon light absorption.

[1] Hayashi, T., Matsuura, A., Sato, H. & Sakurai, M. *BIOPHYSICS*, 8, 115–125 (2012).