Publications

[1] J. Ohnuki, T. Sato, and M. Takano, Piezoelectric allostery of protein, *Phys. Rev E*, **94**, 012406 (2016).

[2] K. Umezawa, J. Ohnuki, J. Higo, and M. Takano, Intrinsic disorder accelerates dissociation rather than association, *Proteins*, **84**, 1124–1133 (2016).

[3] T. Sato, J. Ohnuki, and M. Takano, Dielectric allostery of protein: response of myosin to ATP binding, *J. Phys. Chem. B*, **120**, 13047-13055 (2016).

Presentations

[1] Y. Mizuhara, D. Parkin, and M. Takano, Critical role of cutoff parameter to calculate effective Born radii in simulating protein-protein interaction, Protein Electrostatics, Berlin, Jul. 19, 2016.

[2] J. Ohnuki, T. Sato, and M. Takano, Piezoelectric allostery of protein, Protein Electrostatics, Berlin, Jul. 19, 2016.

[3] K. Tezuka, R. Kiyama, D. Yamakoshi, D. Parkin, and M. Takano, Analysis of the ion pathway of Fo molecular motor using the revised structure with tilted a-subunit helices., BSJ 54th Annual Meeting, Tsukuba, Nov. 18, 2016.

[4] R. Moritake, T. Sato, Y. Suzuki, and M. Takano, Physical mechanism of introducing positive supercoils into bubble DNA by reverse gyrase, BSJ 54th Annual Meeting, Tsukuba, Nov. 18, 2016.

[5] D. Parkin, Y. Mizuhara, and M. Takano, Physical understanding and computational guideline for the balance between Born and Coulomb energies, BSJ 54th Annu. Meeting, Tsukuba, Nov. 18, 2016.

[6] T. Sato, T. Sasaki, J. Ohnuki, and M. Takano, Local dielectric environment around myosin, BSJ 54th Annual Meeting, Tsukuba, Nov. 18, 2016.

[7] J. Ohnuki, T. Sato, H. Okamura, T. Q. P. Uyeda, and M. Takano, Piezoelectric property of an actin filament, BSJ 54th Annual Meeting, Tsukuba, Nov. 18, 2016.

Research Summary

• By using the accelerated MD method, we found the piezoelectric allostery in an actin filament.

• By MD simulation, we elucidated another dielectric allostery path caused by the ATP binding.

• By MD simulation, we found an ATP-binding-induced dielectric allostery in a DNA-binding protein.

• By MD simulation, we found the proton translocation pathway in an ATP synthase.

• By using a coarse-grained model and the adaptive umbrella sampling method, we showed that intrinsic disorder of protein accelerates unbinding from the partner protein.

• By using the Onsager-Kirkwood-Fröhlich theory, we showed anomalous properties of water around myosin.