

## Publications

- [1] Y. Mizuhara, D. Parkin, K. Umezawa, J. Ohnuki, and M. Takano, Over-destabilization of protein-protein interaction in generalized Born model and utility of energy density integration cutoff, *J. Phys. Chem. B*, **121**, 4669-4677 (2017).
- [2] J. Ohnuki, A. Yodogawa, and M. Takano, Electrostatic balance between global repulsion and local attraction in reentrant polymerization of actin, *Cytoskeleton*, **74**, 504-511 (2017).
- [3] T. Sato, J. Ohnuki, and M. Takano, Long-range coupling between ATP-binding and lever-arm regions in myosin via dielectric allostery, *J. Chem. Phys.*, **147**, 215101 (2017).
- [4] H. Ozawa, K. Umezawa, M. Takano, S. Ishizaki, S. Watabe, and Y. Ochiai, Structural and dynamical characteristics of tropomyosin epitopes as the major allergens in shrimp, *Biochem. Biophys. Res. Commun.*, **498**, 119-124 (2018).

## Presentations

- [1] J. Ohnuki and M. Takano, Mechano-electrical communications in actin filament, BSJ 55th Annu. Meeting, Kumamoto, Sept. 19, 2017.
- [2] D. Parkin, Y. Mizuhara, and M. Takano, Continuum-model-based dispersion energy calculation for protein-water interaction, BSJ 55th Annu. Meeting, Kumamoto, Sept. 19, 2017.
- [3] T. Sato, T. Sasaki, J. Ohnuki, K. Umezawa, and M. Takano, Enhancement of electrostatic interaction by hydrophobic surface, BSJ 55th Annu. Meeting, Kumamoto, Sept. 19, 2017.
- [4] M. Iijima, T. Sato, R. Moritake, T. Sasaki, and M. Takano, Physical state change in NADPH-cytochrome P450 oxidoreductase in response to the charge state change, BSJ 55th Annu. Meeting, Kumamoto, Sept. 21, 2017.
- [5] D. Yamakoshi, D. Parkin, K. Tezuka, and M. Takano, Computational Analysis of the Brownian rotation of Fo motor, BSJ 55th Annu. Meeting, Kumamoto, Sept. 21, 2017.
- [6] A. Yodogawa, J. Ohnuki, and M. Takano, Counter-ion-induced electrostatic change in actin: the balance between global repulsion and local attraction in reentrant polymerization, BSJ 55th Annu. Meeting, Kumamoto, Sept. 21, 2017.

## Research Summary

- We studied the combination of the generalized Born model and the continuum Lennard-Jones model for the fast and accurate calculation of the protein-protein interaction.
- By using the generalized Born model, we showed that the reentrant-like actin polymerization can be explained by the Coulombic balance between the global repulsion and the local attraction.
- By applying the accelerated MD method to a protein that regulates the electron transfer, we showed that the redox state affects the structural state.
- By MD simulation, we analyzed the rotary Brownian motion of ATP synthase.