

## 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

- タンパク質間相互作用を高速で正確に計算できる Generalized Born モデルと連続体 Lennard-Jones モデルを組み合わせたモデルを考案し、最適パラメータを明らかにした。
- GB モデルを用いたエネルギー計算により、アクチン重合のリエントラント転移が大域静電斥力と局所静電引力のバランスで説明できることを示した。
- AMD 計算により電子伝達タンパク質における酸化還元状態と構造状態のカップリングを明らかにした。
- MD 計算により ATP 合成酵素における回転ブラウン運動の特性を明らかにした。