

## Publications

- [1] J. Ohnuki, T. Sato, T. Sasaki, K. Umezawa, and M. Takano, Reply: Hydrophobic surface enhances electrostatic interaction in water, *Phys. Rev. Lett.*, **123**, 049602 (2019).
- [2] M. Iijima, J. Ohnuki, T. Sato, M. Sugishima, and M. Takano, Coupling of redox and structural states in cytochrome P450 reductase studied by molecular dynamics simulation, *Sci. Rep.*, **9**, 9341 (2019).

## Presentations

- [1] Takano M, “Depolymerization mechanism of actin due to dielectric allostery”, 11th Toyota Riken International Workshop (2019).
- [2] Ohnuki J, Takano M, “Dielectric and piezoelectric allostery of actin and regulation of cofilin binding”, 11th Toyota Riken International Workshop (2019).
- [3] Ohnuki J, Takano M, “pH-dependent charge-state and intermolecular interaction of actin”, 日本生物物理学会第57回年会 (2019).
- [4] Parkin D, Nakagawa G, Yamakoshi D, Takano M, “Free energy landscape for stator-rotor interaction in Fo rotary motor”, 日本生物物理学会第57回年会 (2019).
- [5] Iijima M, Ohnuki J, Sato T, Takano M, “Dielectric allostery in cytochrome P450 reductase on the surface of lipid membrane”, 日本生物物理学会第57回年会 (2019).
- [6] Uchida K, Ohnuki J, Sato T, Takano M, “Validation of second phosphate binding site in myosin studied by molecular dynamics simulation”, 日本生物物理学会第57回年会 (2019).
- [7] Kuroishi K, Yodogawa A, Parkin D, Takano M, “Over-stabilization of protein-protein interaction in solvent accessible surface area model”, 日本生物物理学会第57回年会 (2019).
- [8] 大貫隼, 高野光則 “誘電・圧電応答に基づく分子機械の運動機構”, 第36回強誘電体応用会議 (2020).
- [9] Ohnuki J, Takano M, “Allosteric pathway in protein explored by Ising machine”, International Conference on Network Science NetSci-X (2020).
- [10] Ohnuki J, Sato T, Sasaki T, Umezawa K, Takano M, “Hydrophobic surface enhances electrostatic interaction in water”, 13th Mini-Symposium on Liquids (2019)
- [11] Ohnuki J, Takano M, “Actin depolymerization and cofilin binding induced by dielectric allostery”, 64th Annual Meeting of the Biophysical Society (2020).

## Research Summary

- 水の電気双極子の揺らぎの相関と誘電率を結びつける Stern-Feller 理論を用いて疎水性平板近傍での水の誘電率特性を解析した。Onsager-Kirkwood-Fröhlich 理論に基づく解析結果との比較し、両者の結果がよく一致することを示した。
- Solvent-Accessible-Surface-Area モデルによる疎水性相互作用計算の研究を行った。
- 力発生、エネルギー変換、電子伝達制御、高分子合成を行う分子マシンの長時間 MD 計算を実施し、それぞれの分子マシンの動作機構の研究を行った。