## 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] Ohunuki 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”, 57th Annual Meeting of Biophysical Society of Japan (2019).

[4] Parkin D, Nakagawa G, Yamakoshi D, Takano M, “Free energy landscape for stator-rotor interaction in Fo rotary motor”, 57th Annual Meeting of Biophysical Society of Japan (2019).

[5] Iijima M, Ohnuki J, Sato T, Takano M, “Dielectric allostery in cytochrome P450 reductase on the surface of lipid membrane”, 57th Annual Meeting of Biophysical Society of Japan (2019).

[6] Uchida K, Ohnuki J, Sato T, Takano M, “Validation of second phosphate binding site in myosin studied by molecular dynamics simulation”, 57th Annual Meeting of Biophysical Society of Japan (2019).

[7] Kuroishi K, Yodogawa A, Parkin D, Takano M, “Over-stabilization of protein−protein interaction in solvent accessible surface area model”, 57th Annual Meeting of Biophysical Society of Japan (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

•We analyzed the dielectric property of water near a hydrophobic surface using the Stern-Feller formula, and compared with the result obtained by the Onsager-Kirkwood-Fröhlich formula.

•We studied the Solvent-Accessible-Surface-Area model to accurately calculate the hydrophobic interaction between biomolecules.

•By conducting large-scale MD simulations of molecular machines that perform force generation, energy conversion, electron-transfer regulation, and polymer synthesis, we investigated functioning mechanisms of those molecular machines.