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] 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，京都，2019 年 5 月.

[2] J. Ohnuki, T. Sato, T. Sasaki, K. Umezawa, and M. Takano, Hydrophobic surface enhances electrostatic interaction in water, The 13th Mini-Symposium on Liquids, Okayama, June 2019.

[3] 大貫隼，高野光則，pH-dependent charge-state and intermolecular interaction of actin，日本生物物理学会第 57 回年会，宮崎，2019 年 9 月.

[4] J. Ohnuki, and M. Takano, Dielectric and piezoelectric allostery of actin and regulation of cofilin binding, The 11th Toyota Riken International Workshop, Nagoya, November 2019.

[5] J. Ohnuki, and M. Takano, Allosteric pathway in protein explored by Ising machine, NetSci-X 2020, Tokyo, January 2020.

[6] J. Ohnuki, and M. Takano, Actin depolymerization and cofilin binding induced by dielectric allostery, 64th Annual Meeting of the Biophysical Society, San Diego, February 2020.

Awards

・Young scientist encouragement award in Waseda Univ. Early Bird Program

Research Summary

・We found that actin, which drives cell dynamics by polymerization and depolymerization coupled with ATP hydrolysis, exhibits dielectric and piezoelectric allostery (polarization in distant regions due to the dielectric and piezoelectric property of protein) in response to ATP hydrolysis, applied tension, and pH change.

・By comparing the distributions of the local dielectric constant of water near a hydrophobic surface between an exact formula which considers long-range dipole correlation and a more approximate one, we found that both formulae can detect the dielectric property of the system.

・We applied the combinatorial optimization technique by Ising machine to the strudy of allosteric pathway in proten molecules.