Publications

[1] T. Sato, T. Sasaki, J. Ohnuki, K. Umezawa, and M. Takano, Hydrophobic surface enhances electrostatic interaction in water, *Phys. Rev. Lett*, **121**, 206002 (2018).

[2] M. Takano, Orchestrated electrostatic interactions among myosin, actin, ATP, and water, in "*The Role of Water in ATP Hydrolysis Energy Transduction by Protein Machinery*" (M. Suzuki, ed, Springer, Singapore, 2018), Chap. 8 (pp. 113-122).

Presentations

[1] M. Takano, Coulombic interaction network and novel allostery in molecular machines, 56th Annual Meeting of Biophysical Society of Japan, Okayama, September 2018.

[2] M. Takano, Enhancement of electrostatic interaction by hydrophobic surface, Workshop on hydration and ATP energy, Sendai, March 2019.

[3] J. Ohnuki and M. Takano, Depolymerization mechanism of actin due to dielectric allostery, Biophysical Society 63rd Annual Meeting, Baltimore, March 2019.

[4] J. Ohnuki, Y. Arimura, T. Kono, K. Kino, H. Kurumizaka, M. Takano, Molecular dynamics prediction of the substrate-binding sites and ligation mechanism in poly-α-glutamate synthetase RimK, The Protein Society 32nd Annual Symposium, Boston, July 2018.

[5] M. Iijima, J. Ohnuki, T. Sato, M. Sugishima, and M. Takano, Coupling of the redox and structural states in cytochrome P450 reductase studied by molecular dynamics simulation, The Protein Society 32nd Annual Symposium, Boston, July 2018.

[6] D. Parkin, D. Yamakoshi, and M. Takano, Half channels and unidirectional rotation in the Fo sector of E. coli ATP synthase observed by molecular dynamics simulation, 56th Annual Meeting of Biophysical Society of Japan, Okayama, September 2018.

[7] D. Yamakoshi, D. Parkin, K. Tezuka, and M. Takano, Coupling of protonation state of conserved residues and rotation angle in Fo rotary motor, 56th Annual Meeting of Biophysical Society of Japan, Okayama, September 2018.

[8] K. Uchida, T. Sato, J. Ohnuki, M. Takano, Dielectric allostery of myosin due to ATP hydrolysis, 32th Annual Meeting of Molecular Simulation Society of Japan, Tsukuba, November 2018.

Research Summary

• Onsager-Kirkwood-Fröhlich 理論に基づき疎水性表面近傍での水の誘電率低下を明らかにし、アンブレラサンプリングを用いた平均力ポテンシャル計算によって疎水性表面近傍で静電相互作用が増強されることを明らかにした。

• ミオシン、アクチン、ATP 合成酵素、電子伝達タンパク質（還元酵素）における電荷のインプットに対する誘電応答（誘電アロステリー）の解析を進めた。