Structure, dynamics, and energy flow that govern Heme protein functions: theory and experiments. Session 3SBA at the 57th BSJ Annual Meeting

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Thanks to recent developments in theoretical/computational/experimental techniques, biophysical mechanisms of protein function have been elucidated at atomic detail. In particular, heme proteins provide ideal research targets for biophysicists because of their natural “probe” built in the protein matrix. On the morning of Thursday, 26th September, at the Annual Meeting of the Biophysical Society of Japan, we discussed recent advancement of biophysical studies on heme proteins and the molecular basis of their function.

Our session opened with the talk by Prof. Takahisa Yamato from Nagoya University. He introduced their theoretical model, energy exchange network, in which residue interactions were evaluated in terms of local transport coefficients of energy flow (Leitner and Yamato 2018). This method was applied to the structural transition upon ligand binding to an oxygen sensor protein, FixLH, and the molecular mechanism of its allosteric signaling was discussed (Ota and Yamato 2019).

The second speaker, Prof. Yoshitsugu Shiro from University of Hyogo, detailed the structural complex of nitric oxide reductase (NOR) (Gonska et al. 2018; Gopalasingam et al. 2019) and nitrite reductase (NiR), which allows a smooth transfer of NO from NiR to NOR. The reduction of cytotoxic nitric oxide is biologically important in cells. Furthermore, they have also characterized the chemical mechanism of the NO reduction on the active site of NOR.

The third speaker was Prof. Misao Mizuno from Osaka University. They demonstrated the vibrational energy relaxation processes in heme proteins with high spatiotemporal resolution. They performed picosecond time-resolved anti-Stokes UV resonance Raman spectroscopy on tryptophan, combined with site-directed mutagenesis, and suggested that vibrational energy flow in hemeproteins occurs predominantly via van der Waals atomic contacts (Kondoh et al. 2016; Yamashita et al. 2018).

The fourth speaker was Prof. Ayana Sato-Tomita from Jichi Medical University. To capture photolysis intermediates of MbCO and HbCO, they used (1) X-ray crystallography combined with laser pumping and cryogenic trapping (Tomita et al. 2009), and (2) pump-probe X-ray crystallography (Tomita et al. 2014) using pulsed laser and pulsed X-ray of synchrotron radiation. As a result, they elucidated the ligand migration processes of heme proteins at atomic detail.

The last speaker was Prof. David Leitner from University of Nevada, Reno. By coarse graining energy transport (ET) dynamics from the all atom to residue level, they have identified a relation between conformational dynamics at equilibrium and ET rates across non-bonded contacts (Reid et al. 2018). ET rates thus provide a window into equilibrium dynamics of proteins and entropy associated with the dynamics of the contact. He also discussed energy transport across the interface of a dimeric hemoglobin, where hydrogen bonded contacts of interfacial water play important roles (Leitner et al. 2019).

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References

- Gonska N, Young D, Yuki R et al (2018) Characterization of the quinol-dependent nitric oxide reductase from the pathogen *Neisseria meningitidis*, an electrogenic enzyme. *Sci Rep* 8:3637. <https://doi.org/10.1038/s41598-018-21804-0>
- Gopalasingam CC, Johnson RM, Chiduzu GN et al (2019) Dimeric structures of quinol-dependent nitric oxide reductases (qNORs) revealed

- by cryo–electron microscopy. *Sci Adv* 5:eaax1803. <https://doi.org/10.1126/sciadv.aax1803>
- Kondoh M, Mizuno M, Mizutani Y (2016) Importance of atomic contacts in vibrational energy flow in proteins. *J Phys Chem Lett* 7:1950–1954. <https://doi.org/10.1021/acs.jpclett.6b00785>
- Leitner DM, Yamato T (2018) Mapping energy transport networks in proteins. In: Parrill AL, Lipkowitz KB (eds) *Reviews in computational chemistry*. Wiley, New York, pp 63–113
- Leitner DM, Pandey HD, Reid KM (2019) Energy transport across interfaces in biomolecular systems. *J Phys Chem B* 123:9507–9524. <https://doi.org/10.1021/acs.jpcb.9b07086>
- Ota K, Yamato T (2019) Energy exchange network model demonstrates protein allosteric transition: an application to an oxygen sensor protein. *J Phys Chem B* 123:768–775. <https://doi.org/10.1021/acs.jpcb.8b10489>
- Reid KM, Yamato T, Leitner DM (2018) Scaling of rates of vibrational energy transfer in proteins with equilibrium dynamics and entropy. *J Phys Chem B* 122:9331–9339
- Tomita A, Sato T, Ichianagi K et al (2009) Visualizing breathing motion of internal cavities in concert with ligand migration in myoglobin. *Proc Natl Acad Sci U S A* 106:2612–2616. <https://doi.org/10.1073/pnas.0807774106>
- Tomita A, Nozawa S, Adachi S et al (2014) Structural dynamics measurements of the biological molecule using pump-probe technique. *J Crysrt Soc Jpn* 56:253–258. <https://doi.org/10.5940/jcrsj.56.253>
- Yamashita S, Mizuno M, Tran DP et al (2018) Vibrational energy transfer from Heme through atomic contacts in proteins. *J Phys Chem B* 122: 5877–5884. <https://doi.org/10.1021/acs.jpcb.8b03518>

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