Emergence of Function in Primitive Chemical Networks Out of Equilibrium

Gonen Ashkenasy

Ben-Gurion University of the Negev, Beer Sheva, Israel

Like many other open systems in nature, living organisms are replete with rhythmic and oscillatory behaviour at all levels, to the extent that oscillations have been termed as a defining attribute of life. Recently, we have started to investigate a chief challenge in contemporary Systems Chemistry research,^[1] that is, to synthetically construct "bottom-up" peptide-based networks that display bistable behaviour and oscillations. Towards this aim, we utilize replicating coiled coil peptides, which have already served to study emergent phenomena in complex mixtures. In the first part of this talk, we describe a simulation study on the kinetic behaviour of small networks of coupled oscillators, producing various functions such as logic gates, integrators, counters, triggers and detectors.^[2] These networks can also be utilized to simulate the connectivity and network topology observed for the Kai-proteins circadian clocks, producing rhythms whose constant frequency is independent of the input intake rate and robust towards concentration fluctuations.^[3] Then, in the second part, we disclose a new experimental bistable network, operating far from equilibrium by constantly consuming energy provided from reducing agents.^[4-6] The two recent studies highlight the conditions affording the phase transition that takes place when a chemical system reaches steady state far from equilibrium chemistry, and their role as the driving force for the emergence of new functions.

References:

- 1. "Systems Chemistry" Chem. Soc. Rev. 2017, 46, 2543.
- 2. Wagner et al. J. Phys. Chem. Lett. 2015, 6, 60.
- 3. Gurevich et al. Chem. Commun. 2015, 51, 5672.
- 4. Mukherjee et al. Angew. Chem. Int. Ed. 2015, 54, 12452.
- 5. Wagner et al. ChemPhysChem 2017, 18, 1842.
- 6. Wagner et al. *submitted* 2018; Maity et al. in preparation 2018.