Harnessing Energy in Chemistry: A Theory-Driven Approach

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Nanotechnology is often associated with atomically precise manufacturing of stable, equilibrium structures. However, biology demonstrates that molecular systems can perform dynamic, energy-driven functions such as muscle contraction and active transport. Mastering this nonequilibrium complexity in synthetic systems offers transformative opportunities for creating lifelike chemistry. In my talk, I will demonstrate how theoretical and computational methods enhance our understanding of the physics governing nonequilibrium chemical processes, building on the foundational concept of the Brownian ratchet [1]. Specifically, I will discuss three key advancements: (i) Nonequilibrium thermodynamics offers an insightful framework for rethinking energetics and efficiency in experimental systems [2]; (ii) Graph theory aids in understanding and characterising complex systems [3]; and (iii) simulations of catalysis-driven motors reveal general insights into their operation [4].

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[2] Amano, S., Esposito, M., Kreidt, E., Leigh, D.A.*, Penocchio, E.* & Roberts, B. M. W. Insights from an information thermodynamics analysis of a synthetic molecular motor. *Nat. Chem.* 14, 530–537 (2022).
[3] Penocchio, E.*, Bachir, A., Credi, A., Astumian, R.D.* & Ragazzon, G.*. Analysis of kinetic asymmetry in a multi-cycle reaction network establishes the principles for autonomous compartmentalized molecular ratchets. *Chem* 10, 3644–3655 (2024).
[4] Penocchio, E.*, Gu, G., Albaugh, A. & Gingrich, T.R.*. Power strokes in molecular motors: predictive, irrelevant, or somewhere in between? *J. Am. Chem. Soc.* 147, 1063–1073 (2025).

Biographical sketch: Emanuele Penocchio is a postdoctoral scholar in the Department of Chemistry at Northwestern University. After studying chemistry in Bologna and Pisa, he obtained a Ph.D. in Physics in 2022 from the University of Luxembourg, with a thesis on the non-equilibrium thermodynamics of chemical reaction networks. Emanuele's research focuses on the physical chemistry underlying chemical systems that consume energy to perform functions. He cherishes interdisciplinary dialogue to identify questions that are theoretically interesting and valued by the experimental community—more about Emanuele at https://emanuelepenocchio.github.io/.