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Applications of non-equilibrium thermodynamics to signaling and metabolic pathways DAWEI HU, ENSHENG LIU, JIAN-MIN YUAN, Drexel University — Signaling transduction pathways play important roles in regulating cell functions, such as growth, differentiation, and apoptosis. Metabolic pathways, on the other hand, generate many metabolites utilized by human body. Abnormal regulations of the enzymes and metabolites associated with these pathways may be related to diseases. In view of their importance, we are interested in applying non-equilibrium thermodynamics to investigate the properties and dynamic behaviors of these two types of pathways. The systems of concentration are the MAPK, coupled MAPK-PI3K, and insulin metabolic pathways. In the case of signaling pathways we study the properties of thermodynamic variables, such as the affinities and fluxes of individual reaction steps, as affected by the perturbations of rate constants, protein-protein interactions, and cross talks. In the case of metabolic pathways, we study the system dynamics, the stability of steady states, and the flux-affinity relations as functions of constant inputs and outputs as well as the parameters of feedback loops. Our goals are to shed light on the design principles of the biological pathways and to rank the most vulnerable nodes of these pathways.

Jian-Min Yuan
Drexel University

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