Non-equilibrium Energy Research Center (NERC)
EFRC Director: Bartosz A. Grzybowski
Lead Institution: Northwestern University

Mission Statement*: To understand self-organization in dissipative, far-from-equilibrium systems and to use this knowledge to synthesize adaptive, reconfigurable materials for energy storage and transduction.*

Our efforts encompass development of far-from-equilibrium statistics, dissipation vs. structure relationships, construction of dissipative/metastable materials (including those with internal feedbacks and those that can self-replicate), and networks of dissipative processes giving rise to complex non-equilibrium systems. From a fundamental point of view, understanding the relationship between dissipation and organization/function of matter out of equilibrium is one of the great challenges facing the physical sciences – in particular, general laws describing dissipative systems would not only allow us to understand better the operation of animate matter (as all organisms are dissipative!) but would also identify the rules/requirements under which artificial materials and systems become least dissipative and, therefore, most energetically efficient. An integral part of NERC's vision is to translate such a theoretical description into the design and synthesis of specific non-equilibrium systems: maximally efficient molecular machines and their collections, materials that convert different forms of energy in the least dissipative fashion, networks of chemical reactions working in synchrony to produce desired products in an optimal fashion, as well as systems that exhibit auto-catalysis, self-organization, and self-replication (each of which requires energy input and dissipation). All in all, our aim is to channel and control dissipation and to put the energy thus "saved" to a useful task.

Since the time of Gibbs, equilibrium has become a familiar and powerful concept. Equilibrium structures, systems, and materials are all governed by the principles of equilibrium thermodynamics and correspond to minima of appropriate thermodynamic potentials. Although finding predictive relationships between the interactions acting in an equilibrium system/material and its final structure might be difficult, it is, at least in principle, possible. This convenient situation changes dramatically in systems displaced from thermodynamic equilibrium – either into kinetically trapped states or into states in which the production of entropy (i.e., dissipation of useful energy) directs the emergence of order. Although virtually all animate systems fall into one of these categories, our knowledge of the non-equilibrium (NE) regime is painfully inadequate. This lack of theoretical understanding limits the development of truly non-equilibrium systems and materials. Such materials are of great interest and promise because it is only outside of thermodynamic equilibrium that one can achieve life-like behaviors such as adaptation, feedback, or self-replication. It is only outside of equilibrium that molecular switches can act as true molecular machines, plasmons can catalyze chemical reactions, and multiple chemical reactions can act in synchrony as chemical systems.

NERC is perhaps the first-ever large-scale collaborative research effort devoted to the study and implementation of non-equilibrium systems and materials. The research team assembled within NERC comprises some of the most accomplished scientists in the world with a unique combination of skills ranging from modeling of non-equilibrium phenomena to the synthesis of molecules and materials that can function outside of equilibrium. The uniqueness of the Center lies in bringing all these diverse skills under one research umbrella and combining them into projects that, in the vast majority of cases, involve both theorists and experimentalists. The success of our effort depends crucially on maintaining the proper collaboration (and also balance!) between theory and experiment and also the balance between the individual creativity of the PIs and the programmatic focus. Since non-equilibrium is a very broad concept and its study could easily become a collection of disjoint research projects on various manifestations of dissipative phenomena, the effort of NERC must be – and is – at all times re-assessed and, if necessary, refocused around the most fundamental and the most practically relevant aspects of energy dissipation. The current focus areas are (i) Theory and Model Systems; (ii) Non-equilibrium Materials; and (iii) Networks.

Non-equilibrium material systems exhibit at least two characteristics that make them relevant to energy-related applications: (i) Their adaptability to the energetic "status" of the environment can translate into the ability to harness "waste" energy from the environment. (ii) Because non-equilibrium ensembles necessarily entail spatial thermodynamic gradients, they can direct and/or transduce this energy into useful work.

The identification of general and predictive rules that describe systems far-from-equilibrium remains one of the greatest challenges of modern science. Despite its difficulty, this challenge is certainly worth undertaking – not only for its fundamental appeal but also for the practical promise. Because they can reside in multiple steady-states controlled by the flux of externally delivered energy (chemical, electromagnetic, or thermal), non-equilibrium systems can adapt to changing environmental conditions, adjust the mode of internal organization, and perform different functions depending the state of experimental signals/controls. Creation of such "adaptive" systems and materials that maintain themselves away from thermodynamic equilibrium require multifunctional and adaptive building blocks. Changing the properties of such blocks by external inputs/stimuli can then lead to changes in material's structure and/or function (Figure 1).

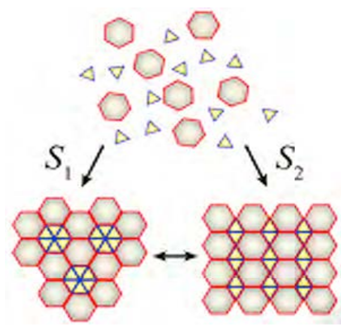

Figure 1. Different stimuli, *S*, evolve the same set of components into different "adaptive" materials.

A cornucopia of creative examples of non-equilibrium systems exist in Nature, many of which are related to energy harnessing (photosynthesis), transport (proticity), or transduction (motor proteins). Our Center's goal is to learn how to use the non-equilibrium phenomena as skillfully and efficiently as Nature does, by thinking about new synthetic systems and supporting this effort by theoretical input and foundation.

Non-equilibrium Energy Research Center (NERC)	
Northwestern University	B.A. Grzybowski (Director), I. Szleifer (Associate Director), C. Mirkin, M.O. de la Cruz, M.A. Ratner, G.C. Schatz, J.F. Stoddart, S.I. Stupp, E. Weiss
Harvard University	G.M. Whitesides
University of Michigan	S.C. Glotzer
The Pennsylvania State University	K.J.M. Bishop
University of Massachusetts Boston	J. R. Green

Contact: Bartosz A. Grzybowski
Professor of Physical Chemistry and Chemical Systems' Engineering
nerc@northwestern.edu
847.467.1295 (Ms. Leah Seiffert, Program Assistant)
www.nercenergy.com