

various Chinese research institutes and universities. In these years, the system was involved in approximately 20 research projects within which several excellent achievements were made. Furthermore, the system donated valuable running time to several national defense projects. The accomplishment of this platform promoted China's competitiveness in this field, and improved the usage efficiency of Beijing Electron Positron Collider (BEPC).

Photoinduced Electron Transfer, Energy Transfer and Chemical Reactions in Supramolecular Systems

Achieved by: Chenho Tung, Lizhu Wu, Liping Zhang, and Bin Chen

Technical Institute of Physics and Chemistry, CAS

Support categories:

1. Key Program Project (No. 20332040 and No. 20333080)
2. National Science Fund for Distinguished Young Scholars (No. 20125207)

The research team led by Prof. Chenho Tung (CAS member) trekked in the research of photoinduced electron transfer, energy transfer and chemical reactions of supramolecular system for 20 years. They honored the 2nd class National Natural Science Award in 2005 and obtained a series of research achievements. This project was devoted to the interdisciplinary area of organic chemistry and physical chemistry, and involves three parts:

1) Microreactor-controlled selectivity in photochemical reactions. The development of efficient and highly selective methods for organic synthesis is one of the main topics in organic chemistry, and much effort has been directed toward this goal. Of various approaches the use of organized and constrained media has shown considerable promise. The scientists of this project have successfully controlled the product selectivity of a variety of photochemical reactions by using molecular aggregates and the cavities and surfaces of microporous solids as microreactors. For example, they synthesized a series of large-ring compounds in high yields under high substrate concentrations in microreactors (*Acc. Chem. Res.* 2003, 36, 39; *J. Am. Chem. Soc.* 1998, 120, 11594; *J. Org. Chem.* 1996, 61, 9417; 1999, 64, 5156; *Org. Lett.* 2001, 4, 1175). In the photosensitized oxidation of alkenes, they could direct the oxidation selectively toward either the singlet oxygen mediated or the superoxide radical anion mediated products by controlling the status and location of the substrate and sensitizer molecules in the reaction media (*Pure. Appl. Chem.*

2000, 72, 2289; *J. Am. Chem. Soc.* 1998, 120, 5179; 1998, 120, 11874; 2000, 122, 2446; *Chem. Comm.* 2000, 1085; *Chem. Comm.* 2001, 2280). They also could control the regioselectivity in the cycloaddition of 9-substituted anthracenes, and the photocyclization of azobenzene and stilbazole by using microreactors (*J. Org. Chem.* 1998, 63, 5857; *Org. Lett.* 2003, 5, 1075; *Tetrahedron. Lett.* 2002, 43, 1281.)

2) Photoinduced intramolecular long-distance electron transfer and energy transfer. Photoinduced electron transfer and energy transfer play an important role in chemical and biochemical processes. Electron transfer and triplet energy transfer in general require proximity of the donor and acceptor comparable to their van der Waals radii. However, the evidences for long-distance electron transfer and triplet energy transfer have been accumulated. In this project the scientists have provided a series of evidences for photoinduced intramolecular long-distance electron transfer and energy transfer via a "through-bond" or a "through-space" mechanism. They utilized androstene skeleton or crown ether moiety as bridges, mounted an antenna chromophore (benzidine, benzophenone, carbazole, dibenzolmethanoboron difluoride etc.) and a norbornadiene (or quadricyclane) group on the bridge framework, and investigated photoinduced intramolecular triplet energy transfer and electron transfer within these systems. They demonstrated that electron transfer and triplet energy transfer processes occur with reasonably large rate constants via a "through-bond" or a "through-space" mechanism depending very much on the nature of the bridge, although the donor and acceptor are separated as far as by ca. 20 Å (*J. Am. Chem. Soc.* 1997, 119, 5348; *J. Phys. Chem.* 1996, 100, 4480; *J. Phys. Chem. A.* 2003, 107, 3438; *Chem. Eur. J.* 2003, 9, 2763). They assembled a series of donor-sensitizer-accepter systems and obtained long-lived photoinduced charge-separation (*J. Phys. Chem. B.* 2000, 104, 9468). They also utilized the metal-to-ligand charge transfer excited state of platinum (II) terpyridyl complexes as the photocatalyst successfully to produce hydrogen in homogeneous solution (*J. Am. Chem. Soc.* 2004, 126, 3440).

3) Hydrophobic and lipophobic effects on photochemical and photophysical processes. Hydrophobic and lipophobic interactions are important intermolecular interactions. The scientists of this project have provided a series of evidences for aggregate formation and self-coiling of molecules with non-polar chains in mixed

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organic-aqueous solvents. They also demonstrated that molecules with polar regions tend to associate and self-coiling in non-polar solvents. The driven force in the later case is lipophobic interactions. They provided the examples for application of lipophobic interactions to expedite the formation of macrocyclic entities (*J. Am. Chem. Soc.* 1990, 112, 6322; *J. Chem. Soc. Chem. Commun.* 1989, 1891; *J. Chem. Soc., Faraday Trans.*, 1994, 90, 947; 1995, 91, 2671; 1994, 92, 1381; *J. Phys. Chem.* 1995, 99, 8311; *Tetrahedron Lett.* 2001, 42, 9249).

To summarize, the scientists of this project have made great achievements in their study on physical organic chemistry and supramolecular chemistry, as evidenced by their near 100 high level publications, among which 1 appeared in *Acc. Chem. Res.*, and 7 in *J. Am. Chem. Soc.* They have given over 50 invited or plenary lectures at international conferences such as Gordon Conference on Supermolecules and Assemblies (1993), Gordon Conference on Organic Photochemistry (1993), 17th IUPAC Symposium on Photochemistry (1998), 15th IUPAC Conference on Physical Organic Chemistry (2000), etc. The paper published in *Acc. Chem. Res.* has been translated into Japanese by Japanese scientists and republished in Japanese journal *Expected Material for the Future*.

Evolutionary Computation and its Application

Achieved by: Licheng Jiao¹, Lishan Kang², Zhenya He³, and Tao Xie⁴

1. Xidian University, China

2. Wuhan University, China

3. Southeast University, China

4. National University of Defense Technology, China

On Mar. 23, 2006, a project in the Major Program of NSFC – “Evolutionary computation and its application”, managed by Prof. Licheng Jiao, Prof. Lishan Kang, Prof. Zhenya He, and Prof. Tao Xie, passed its Final Qualification Process and was evaluated as Excellent.

Through a 4-year research effort, the project team progressed in theories, methods and applications of evolutionary computation. They set up a basic computation framework for clonal selection, systematically studied immunological system mechanisms such as adaptivity, chaos property, immunological memory, immunological forgetting, immunodominance, non-Darwinian evolution and so on. And further they proposed a series of clonal selection algorithms. The convergence, complexity and parameter variations

of these algorithms were detailedly analyzed. Moreover, they outlined a model for synergistic co-evolutionary computing, and set up a multi-agent evolutionary computing framework. Once they were put into practice, varieties of algorithms were also designed targeting on mass data analysis, numerical optimization, and combinatorial optimization. The convergence of those freshly designed algorithms was guaranteed. Based on above evolutionary and clonal algorithms, they put forward quantum evolutionary computation and quantum clonal selection computation algorithm frameworks. Their convergence, complexity, and parameter variations were also analyzed. Then, they set up a theoretical system for the modeling and optimization for a paralleled evolutionary computing system. The system convergence was verified; and its complexity theorem for automatic program design in evolutionary modeling was outlined. They hold various Chinese patents on mass data classification, equation optimization, TSP problem, N-queen problem, N-dim 0-1 bag problem, SAT problem, multi-user detection in communication network, multicast routing, system approximation, VLSI design, image processing etc. Their breakthrough work in mass data classification and VLSI design were published in *IEEE Transactions on Evolutionary Computation*. In the optimization of high dimension equations, their solutions for ten-thousand-dimension equation and 107-queen problem were fixed in linearized and approximately linearized time complexity respectively. These approaches were much better than others. In the same time, the project team resolved 6 challenging problems including dynamic multi-target TSP problem, automatic program design for evolutionary modeling, million-dimension Bump problem, point distribution on sphere surface, multi-target equation optimization, and multi-layer and multi-scale dynamic modeling problem. The related results were published in *Evolutionary Computation*. They also designed new evolutionary neural network models and algorithms in transient evolutionary chaos neural network, stability analysis of neural network, evolutionary neural network trees, evolutionary supporting vector machine, evolutionary blind deconvolution & nonlinear kinetics as well as cryptic communication etc. These new ideas were successfully utilized in channel assignment, satellite broadcast scheduling, image processing, biomedical signal processing, security analysis on encryption algorithm, multi-target optimization etc.