

Photoinduced Proton Transfer in Chemistry and Biology

What is the latest news in the field of photoinduced proton transfer (PPT)? This elementary step is obviously one of the most fundamental reactions in nature. However, understanding the way in which the environment mediates proton dynamics remains a fundamental challenge in chemistry and biochemistry and continues to be an area of active experimental and theoretical investigation. Ever since the first appearance of photoinduced proton transfer in the late 1940s, numerous efforts have been made in understanding its fundamental behaviors as well as looking into practical and future applications. Several themed collections and special issues related to photoinduced proton transfer have been published since 2000, and PPT-related meetings are organized periodically. To the best of our knowledge, the last PPT-themed journal issue was the themed issue “Hydrogen bonding in electronically excited states” (*Phys. Chem. Chem. Phys.* **2012**, *14*, 8753–9236), edited by Guang-Jiu Zhao and Ke-Li Han. The last PPT-related conference was the Gentner symposium on “Proton Mobility in Chemical and Biological Systems” at Ma’agan Holiday Village, Israel, organized on February 7–12, 2010, by Noam Agmon and Shy Arkin. Worth noting are much smaller biennial Telluride workshops “Proton Transfer in Biology” which often include talks on the PPT in biological systems.

This was the first time the specific title “Photoinduced Proton Transfer in Chemistry and Biology” was used for a symposium session in the ACS National Meeting. This symposium was organized by the Division of Physical Chemistry at the 248th American Chemical Society National Meeting in San Francisco, CA, on August 10–14, 2014. This special issue of the *Journal of Physical Chemistry B* is based on (but not limited to) the symposium activities.

A very broad spectrum of PPT-related problems brought together more than 80 leading specialists from 17 countries all over the world. In this five-day gathering, 65 talks and 22 posters were presented. We were thankful to the presenters for submitting their papers to this special issue. The symposium topics included the modern PPT theory (presented by Hynes, Laurent, Olsen, Sobolewski, Thiel, Hammes-Schiffer, Rega, Slipchenko, Popov, Robert, and Pines), the synthesis of novel photoacids and photobases (Tolbert, Gryko, and others) and their ultrafast studies (Huppert, Lustres, Kwon, Mohammed, Vauthey, Petersen, Htun, and Nibbering), the PPT studies in the wide array of systems including proteins (Shcherbakova, Fang, Solntsev, Mely, Nemukhin, Chou, Agmon, Boxer, Moore, Kim, Amin, and Barry), metal complexes (Wenger), DNA (Shafirovich, Kohler, and Temps), polymers (Vaganova), microheterogeneous systems and inclusion complexes (Douhal and Levinger), and the gas phase (Zwier, Sekiya, Jouvét, Fujii, and Cheng). Finally, numerous PPT applications were discussed. They included a utilization of PPT for the understanding of the bioluminescence color tuning (Naumov, Rhee, and da Silva), in the reversible and irreversible pH jumps using the transient photoacids and PAGs (photoacidic generators) (Yao, Jullien, Aoyagi, and Glusac), photochromism

(Sliwa), apoptosis studies (Bhattacharyya), singlet oxygen monitoring (Nagaoka), and molecular pixels development (Park). This symposium attracted people not only from the physical chemistry division but also a lot of theoreticians, biochemists, and organic and material chemists demonstrating an equivocal importance of the subject, and it was heavily attended throughout the five-day series of sessions. The abstracts of the talks can be found online at the Past National Meetings Technical Programming Archive at the ACS Web site.

The symposium and this special issue also had the purpose of celebrating the birth anniversaries of the former Ph.D. (80th for Prof. Michael G. Kuzmin, Moscow State University) and postdoctoral (70th for Prof. Dan Huppert, Tel-Aviv University, and 65th for Prof. Laren M. Tolbert, Georgia Tech) advisors for one of us (K.M.S.). These scientists brought a seminal contribution to the PPT studies in the past 50 years and are still the active players in the field! Michael Kuzmin was the first Soviet/Russian photochemist who developed a deep understanding of the relation between the kinetics and thermodynamics in PPT. He also discovered a competition between the adiabatic and nonadiabatic PT steps. Dan Huppert, an expert in ultrafast spectroscopy, revealed the molecular mechanism of the PPT at various time scales and free energy regimes. Laren Tolbert, an organic chemist by training, developed a new class of “super” photoacids that make possible the studies of intermolecular PPT in nonaqueous solvents. We are happy to have their contribution in this issue.

We hope that the readership finds this special issue inspiring and the new insights into PPT can be shared among the interdisciplinary research fields.

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