

Final Narrative Report - Award Number DE-SC-0013798

“Structure and dynamics in complex chemical systems: Gaining new insights through recent advances in time-resolved spectroscopies,” a symposium on cross cutting challenges on the chemical dynamics of heterogeneous systems

This award from the U.S. Department of Energy Office of Science, Office of Basic Energy Sciences (CPIMS Program) provided funds (\$5100) to the Division of Physical Chemistry for partial support of a symposium entitled “**Structure and dynamics in complex chemical systems: Gaining new insights through recent advances in time-resolved spectroscopies**” within the program of the 250th National Meeting of the American Chemical Society in Boston, MA. This symposium was co-organized by Arthur Bragg (Johns Hopkins University, Chemistry), Amber Krummel (Colorado State University, Chemistry), and Poul Petersen (Cornell University, Chemistry).

Summary of symposium schedule and participation. A copy of the official symposium program is appended to this narrative. The symposium was held between Sunday August 16th and Thursday August 20th as eight half-day sessions (8:00-11:40 am Sunday-Wednesday; 1:20-4:50 pm Sunday, 1:20-4:30 pm Monday, and 1:20-5:25 pm Wednesday; 8 am-noon Thursday). Each half-day session included 3-4 invited talks (35 min. duration, including discussion) and 2-4 contributed talks (20 min. duration, including discussion); each session was split with a 20-min. break. In total, this symposium included presentations from 29 invited and 22 contributed speakers. The list of invited speakers for this symposium matched the original list of proposed invited speakers with few substitutions. Contributed talks were selected from a publicized open call for abstract submissions from the Division of Physical Chemistry. All but two abstracts submitted in response to this call were accommodated with contributed talks; those two were recommended for the general Physical Division poster session as they were far outside of the scope/theme of this symposium. Two contributed submissions from post-doctoral researchers were promoted to invited-talk duration in recognition of their running for the *Journal of Physical Chemistry* Award for Post-doctoral Research Excellence. The official schedule was executed as planned with only two late withdrawals due to illness and travel-related problems (one each invited and contributed talk). More than half of the presenters (26 of 51) were at the rank of assistant professor, post-doctoral researcher, or graduate student. 8 of the 29 invited presenters were female scientists (a 9th could not speak due to illness); 1 contributed presentation was from a female PI, with another presented by a post-doctoral researcher from the group of a female PI. On average there were over 50 attendees per session, with 60 attendees on Sunday and over 40 attending the final session on Thursday morning.

Summary of symposium thematic organization. This symposium was organized specifically to foster dialog on recent progress towards meeting challenges associated with the interrogation of dynamics in complex chemical systems (including many directly relevant to national interests in energy) through the application and further development of novel spectroscopic methods. The organizers gathered experts in these various subfields to share their perspective and advances towards elucidating chemical dynamics in various environments. The final symposium program was organized according to the following topical areas (organized generally by system type, environment, or methodology):

- 1) Interfacial Phenomena
- 2) Liquid Environments

- 3) Photophysical Dynamics of Biological and Biomimetic Systems
- 4) Biological Interfaces and Interactions
- 5) Interfacial Phenomena in Materials
- 6) Structure, Dynamics, and Behaviors of Material Systems
- 7) New Techniques

Summary of symposium goals and indicators that they were met.

The proposed goals of this symposium included:

(1) *Providing a forum for spreading or cross-fertilizing conceptual and technical developments for interrogating and understanding heterogeneous chemical systems across boundaries of various subfields.* This symposium met this goal by scheduling topics of mutual interest to various subfields that led to overlapping attendance. For example, a session on interfacial properties of materials was scheduled as a bridge between sessions on aqueous and biological interfaces early in the week and materials later in the week, and led to attendance from both research communities. In other instances, sessions on other topics were interleaved to ensure cross-fertilizing dialog.

(2) *Inspiring both young and established scientists alike to take on these problems with new approaches and excitement.* 26 of the 51 presenters at this symposium were at the rank of assistant professor, post-doctoral researcher, or graduate student; 5-6 presenters were at the rank of associated professor, with the remaining (~20) at rank of full professor. This symposium met this goal with this balanced age/rank distribution and a sustained attendance of both young and established scientists for each other's presentations throughout the week.

How support was applied. This award enabled the second goal of this symposium, as it was used specifically to partially reimburse registration costs for young scientists participating in the symposium. [ACS early-bird registration fees at the time of the meeting were \$390 for members and \$200 for graduate-student members.] Funds received from this award were used specifically to refund \$125 each in registration fees for 5 contributing graduate and post-doctoral presenters from (domestic) institutions located within the Boston area (the meeting location); roughly \$300 each in registration fees for 7 contributing post-doctoral presenters from non-local domestic institutions; and roughly \$300 each in registration fees for 8 presenters at the Asst. Professor level from non-local domestic institutions (3 contributing, 5 invited). ***NONE OF THIS SUPPORT WAS USED FOR PURCHASE OF EQUIPMENT, SUPPLIES, OR REAL ESTATE.***

Relevance to the DOE-BES and CPIMS missions. As a whole, this symposium provided a forum for discussing first-principle understandings of molecular reactivity and dynamics in a range of complex condensed phase environments, such as solutions and interfaces, driven by energy-relevant chemical, physical, electron- and photon-driven processes. This symposium highlighted how chemical environment influences chemical structure and reactivity. Furthermore, this symposium provided a forum for discussing methods for interrogating and interpreting structure-dynamics relationships using novel techniques that may be applied across disciplines. These challenges are at the heart of the CPIMS and DOE missions. Finally, the support provided was used explicitly to fund attendance of young scientists contributing to these discussions, thereby promoting the future of research on these topics that are critical for novel energy utilization and future energy security of the United States.