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Final Report for Department of Energy Project:

“Support for the 2024 American Conference on Theoretical Chemistry (ACTC)”
Project Number DE-SC0024993

Final Report
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Project Summary/Abstract: Funds are requested in support of the 2024 American Conference on Theoretical Chemistry. Funds are being requested from the Department of Energy in support of conference registration fees for graduate student and post-doctoral researcher registration fees. This conference will be held in North Carolina, and between 200 and 250 participants are expected. This is the major North American meeting of theoretical chemists, showcasing diverse developments in all aspects of modern theory, including methods development and applications. Applications span all aspects of chemistry, biochemistry, and materials science, including important applications to energy science. The conference will include four days of seminars and poster sessions. As well as serving as a meeting ground for sharing scientific developments and discoveries, the meeting also serves as a locus for mentoring and career development involving younger scientists. The meeting will be chaired by Prof. David Beratan of Duke University, and he will be assisted by other faculty from the region: Profs. Weitao Yang (Duke), Patrick Charbonneau (Duke), Yosuke Kanai (University of North Carolina - Chapel Hill), Zhiyue Lu (University of North Carolina - Chapel Hill), and Elena Jakubikova (North Carolina State University). This group will form a conference committee that will define thematic topics for the conference, will invite speakers, and will assist with running the conference.

The 2024 American Conference on Theoretical Chemistry was held very successfully June 17-24, 2025. Over 270 participants were in attendance. The scientific program appears here: <https://www.actc2024.org/programme>, and the conference included over 40 lectures on theoretical chemistry. In addition to our extensive technical talks, we also had sessions that focused on topics of broader interest to the community including: history and philosophy of theoretical chemistry, frontier experimental challenges facing theory, journals/funding agencies/infrastructure, and frontiers of computing. Most participants at the conference were graduate students and post-doctoral associates, with some undergraduate participants as well. The DOE support was used largely to defray the costs for these young scientists to participate in the conference. The meeting was held at the University of North Carolina at Chapel Hill and the students were housed in the dormitories on campus; the scientific sessions and supported meals were at the Carolina Inn on the campus. Highlights of the conference included inspirational lectures from two Nobel Prize winners in the field of theoretical chemistry and multiple sessions on energy science and catalysis. The response to the participants to the content of the meeting and to the venue was extremely positive. The next meeting of this group will occur in 2027.