PROMOTION RECOMMENDATION The University of Michigan College of Literature, Science, and the Arts

Paul M. Zimmerman, associate professor of chemistry, with tenure, College of Literature, Science, and the Arts, is recommended for promotion to professor of chemistry, with tenure, College of Literature, Science, and the Arts.

Academic Degrees:

Ph.D.	2010	Stanford University
B.A.	2005	University of California, Berkeley

Professional Record:

2018-present	Associate Professor, University of Michigan
2012-2018	Assistant Professor, University of Michigan

Summary of Evaluation:

<u>Teaching</u>: Professor Zimmerman has taught two different courses since tenure: Chem 260 and Chem 571. Chem 260 is an entry level physical chemistry course required for majors with enrollments typically in the 80-100 range. This course was new for Professor Zimmerman since promotion. Chem 571 is Quantum Chemistry, a core course for our physical chemistry graduate students. In both cases his student evaluations were good and comparable to those of other professors who have taught the course. He has worked well to engage students in his classes even during the transition to online courses. His colleagues working with him on these courses have valued his work. As a research advisor, Professor Zimmerman currently has twelve graduate students (another ten already graduated), three undergraduates, and two post-doctoral scholars under his mentorship. He has graduated ten Ph.D. students. His mentoring is considered a strength. He has a large number of students, and they are consistently publishing well and obtaining excellent placements.

<u>Research</u>: Professor Zimmerman develops and applies quantum mechanical theory to study many aspects of chemistry, including: reaction prediction; electronic structure determination of molecules; design of light-harvesting molecules; and mechanical processing of polymers. Given the challenges of solving quantum mechanical equations, Professor Zimmerman, like many theorists, is developing approximations that can reduce computing cost to solve problems. Professor Zimmerman's most productive research thrust has been developing and applying methods to determine reaction mechanisms and pathways. Another theme has been in electronic structure calculations. As electronic structure governs reactivity and interactions with light among other important properties, it is a fundamental goal of theory to accurately calculate such structures. Density functional theory has been the mainstay approach, but it only works for simple systems. Since his last promotion, he has made advances in further developing "incremental full configuration interaction" or iFCI, and achieved accuracy comparable to other methods at a fraction of the computational cost, allowing calculation of electronic structure of large molecules with over eighty electrons. He has also developed theory that has guided processing of polymers for recycling and expanded his work on computing important electronic state changes for photoactive materials, used for solar energy conversion among many other technical goals.

Professor Zimmerman has been highly productive, with thirty-eight papers published since his last promotion that are a mix of computational advances and collaborative applications of his methods. He has been well funded, with several new grants since his last promotion, and opened new research vistas related to mechanochemistry and computational methods while significantly augmenting the several research thrusts developed pre-tenure. These are indicators of excellent prospects for growth and future success. He has developed an outstanding international reputation, especially for reaction discovery and prediction.

Recent and Significant Publications:

- Kim, H., Keller, B., Ho-Wu, R., Abeyasinghe, N., Vazquez, R. J., Goodson III, T., & Zimmerman, P. M. (2018). Enacting two-electron transfer from a TT state of intramolecular singlet fission. *Journal of the American Chemical Society*, 140(25), 7760– 7763.
- Rask, A. E. & Zimmerman, P. M. (2021). Towards full configuration interaction for transition metal complexes. *Journal of Physical Chemistry A*, 125(7), 1598-1609.
- Dang, D.-K. & Zimmerman, P. M. (2020). Fully variational iCASSCF. Journal of Chemical Physics, 154(1). https://doi.org/10.1063/5.0031208
- Sati, G., Martin, J., Xu, Y., Malakar, T., Zimmerman, P. M. & Montgomery, J. (2020). Fluoride migration catalysis enables simple, stereoselective, and iterative glycosylation. *Journal of the American Chemical Society*, 142(15), 7235-7242.

<u>Service</u>: Professor Zimmerman's service includes committee and DEI work at the department and university level as well as reviewing and workshop organizing for the external community. His most significant service has been leading the department's industrial relations committee where he helped facilitate collaborations between faculty and Merck and P&G. He volunteered to be trained to run "by-stander intervention" workshops so that our department can host this program regularly for our graduate students. He serves on the management committee of the Michigan Institute for Computational Discovery and Engineering. He co-organized an NSF sponsored Innovation Lab that resulted in feedback to NSF for research directions, collaborations, and proposal concepts.

External Reviewers:

Reviewer (A): "Within his peer group, I consider Professor Zimmerman to be among the very top in North America, if not worldwide."

Reviewer (B): "Professor Zimmerman is an excellent scientist, teacher and citizen of our community and I do enthusiastically recommend him for promotion to the rank of Full Professor"

Reviewer (C): "I am very impressed with Professor Zimmerman's approach to research. He develops new important and useful theoretical methods that are designed to address challenging problems in the chemical sciences"

Reviewer (D): "It is very clear to me that Paul Zimmerman is an extraordinarily versatile scientist, expert in advanced quantum mechanics, dynamics, machine learning, making important contributions to synthesis, and has made a mark in the development of robust methods to explore reaction surfaces. Zimmerman is a brilliant computational chemist..."

Reviewer (E): "Since achieving tenure at U of Michigan, Zimmerman has been impressively productive...He is widely recognized nationally in the chemistry community and his work is well regarded."

Reviewer (F): "I consider Professor Zimmerman to be one of the leading voices, in a global scale, helping to shape the future of theoretical and computational chemistry."

Summary of Recommendation:

Professor Zimmerman has developed creative advanced computational methods for studying a wide array of significant chemistry problems, developed an appropriate teaching portfolio and mentored an exceptional number of advanced students with success, and contributed service to enhance industrial collaboration and computational education on campus. The Executive Committee of the College of Literature, Science, and the Arts and I recommend that Associate Professor Paul M. Zimmerman be promoted to the rank of professor of chemistry, with tenure, College of Literature, Science, and the Arts.

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Anne Curzan, Dean Geneva Smitherman Collegiate Professor of English Language and Literature, Linguistics, and Education Arthur F. Thurnau Professor College of Literature, Science, and the Arts

May 2022