



EMERSON CENTER LECTURESHIP AWARD SYMPOSIUM



C. L. EMERSON

EMERGING COMPUTATIONAL AND QUANTUM APPROACHES

October 23rd, 2026
Atwood Hall, Room #360

AWARD WINNER &
KEYNOTE SPEAKER

Prof. Laura Gagliardi,
The University of Chicago

Learning Multireference Chemistry: Accurate Models for Excited States and Dynamics



Addressing complex yet practical problems in natural sciences requires an accurate description of near-degenerate, low-lying electronic states. This challenge makes multireference electronic structure methods indispensable, although their broader application remains limited by computational cost and difficulties of controlling electronic structure under varying reaction conditions and dynamics. I will discuss recent progress toward making multireference methods more practical, systematic, and transferable, illustrating this through: (a) methane C–H activation at metal–oxo sites in metal–organic framework nodes, and (b) machine learning potentials trained on multireference electronic-structure data in combination with the weighted active space protocol. This approach is applied to the challenging TiC^+ -catalyzed methane C–H activation.

INVITED SPEAKERS

EVENTS SCHEDULE

	1:00 – 1:30	OPENING CEREMONY & AWARD PRESENTATION
	Laura Gagliardi University of Chicago	1:30 – 2:30 <i>Learning Multireference Chemistry: Accurate Models for Excited States and Dynamics</i>
	Jesse McDaniel, Georgia Institute of Technology	2:30 – 3:15 <i>Computational Electrosynthesis and Development of Novel DFT-QM/MM Algorithms and Software</i>
	3:15 – 3:30	Coffee Break
	Francesco Evangelista Emory University	3:30 – 4:30 TBA
	Lili Wang Emory University	4:30 – 5:15 <i>Spin Relaxation and Coherence in Low-Dimensional Lead Halide Perovskites and Nanocrystals</i>
	Nicholas Mayhall Indiana University	5:15 – 6:00 <i>Molecular simulation with quantum computers</i>
	6:00 – 6:10	CLOSING
	6:30 – 9:00	DINNER (by invitation)

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