Chemical reactions as switchable networks in condition's hyperspaces

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ABSTRACT: My talk will narrate the two ongoing revolutions reshaping organic chemistry – by algorithms and by robots. Historically, problems ranging from synthesis planning to the discovery of new reactions have been an exclusive domain of human intellect and/or dexterity of human experimentalists. This has now changed and both tasks are performed not only faster but also better by algorithms, robots or even robots guided with chemical AI algorithms. In particular, these approaches challenge our understanding of chemical reactions – instead of single-line equations (A + B \rightarrow C), algorithms and robots allow us to explore reactions as dynamic networks embedded in multidimensional "hyperspaces" of conditions, where control parameters can "switch" the system between different and often unexpected major products. My lecture will showcase some of these discoveries and their reduction to practice. A new age of chemistry has dawned, with profound repercussions for how we conceptualize and execute organic synthesis.

KEY REFERENCES including the last one to be published on the day of the lecture:

- 1. Nature **588**, 83–88 (**2020**), https://doi.org/10.1038/s41586-020-2855-y
- 2. Science **369**, eaaw1955 (**2020**), https://doi.org/10.1126/science.aaw1955
- 3. Nature **604**, 668–676 (**2022**), https://doi.org/10.1038/s41586-022-04503-9
- 4. Science **378**, 399–405 (**2022**), https://doi.org/10.1126/science.adc8743
- 5. Nature **625**, 508–515 (**2024**), https://doi.org/10.1038/s41586-023-06854-3
- 6. Science **384**, eadk9227 (**2024**), https://doi.org/10.1126/science.adk9227
- 7. Nature (**2025**), https://doi.org/10.1038/s41586-025-09490-1