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BIO: Bartosz A. Grzybowski is a Distinguished Professor of Chemistry at UNIST and a Director of the IBS Center for Algorithmic and Robotized Synthesis (CARS). He is also Professor at the Institute of Organic Chemistry, Polish Academy of Sciences. Although he has spent a large fraction of his research career on esoteric problems of self-assembly and non-equilibrium systems, he considers his most impactful discoveries to be in the area of computer-driven synthesis (e.g., the Chematica/Synthia and Allchemy programs). Grzybowski is an author of ca. 300 articles, and over the years received numerous accolades of which the 2016 Feynman Prize and the 2022 Foundation for Polish Science Prize are closest to his heart. He started several companies – most recently, Allchemy, Inc. – and has advised various industrial and governmental bodies in areas ranging from AI to oil drilling.

TALK

Title: Synthesis planning, mechanistic analysis and discovery of new reaction classes in the age of computers

Abstract: After decades of rather unsuccessful attempts, computers are finally making impact on the practice of synthetic chemistry. This change is made possible by the combination of increased computing power and, above all, new algorithms to encode and manipulate synthetic knowledge at various levels, from sequences of full reactions to sequences of mechanistic steps. In my talk, I will illustrate how these advances have enabled completely autonomous planning of multistep syntheses of complex (natural product) targets, how they allow us to elucidate complex reaction mechanisms and, above all, discover new classes of reactions.

Relevant references

1. B. Mikulak-Klucznik *et al.* Computational planning of the synthesis of complex natural products. *Nature*, **588**, 83-88 (2020)
2. A. Wołos *et al.* Synthetic connectivity, emergence, and self-regeneration in the network of prebiotic chemistry. *Science* **2020**, *369* (6511).
3. A. Wołos *et al.* Computer-designed repurposing of chemical wastes into drugs. *Nature* **604**, 668-676 (2022).
4. T. Klucznik *et al.* Computational prediction of complex cationic rearrangement outcomes. *Nature* (2023) https://doi.org/10.1038/s41586-023-06854-3.