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BIO: Bartosz A. Grzybowski is a Distinguished Professor of Chemistry at UNIST and a Group Leader at the IBS Center for Soft and Living Matter. 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, processes and reaction discovery 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 impact discovery pipelines and processes related to medicinal and circular chemistries, and how they allow us to elucidate reaction mechanisms and, above all, discover new classes of reactions.

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