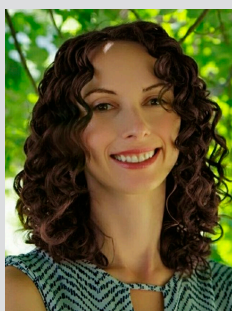


Young Career Focus: Professor Adelina Voutchkova-Kostal (George Washington University, USA)

Background and Purpose. SYNFORM regularly meets young up-and-coming researchers who are performing exceptionally well in the arena of organic chemistry and related fields of research, in order to introduce them to the readership. This Young Career Focus presents Professor Adelina Voutchkova-Kostal (George Washington University, USA).

Biographical Sketch



Prof. A. Voutchkova-Kostal

Adelina Voutchkova-Kostal received her B.A. in Chemistry and Biochemistry from Middlebury College, USA (2004), and her M.Sc. and Ph.D. (2009) from Yale University (USA) under the guidance of Bob Crabtree. She continued her post-graduate work at the Yale Center for Green Chemistry and Green Engineering (USA) with Paul Anastas and Julie Zimmerman, focused on the rational design of safer chemicals. She launched her independent career in the Chemistry Department at George Washington University (Washington, DC, USA) in 2012 and is currently an Associate Professor. Her research program is focused on the design of catalytic processes that can help facilitate circular economies. The catalytic systems being developed cross the boundaries of homogeneous and heterogeneous catalysis, and consider lifecycle and hazard factors. The group is also involved in development of tools for designing safer commercial chemicals in collaboration with computational chemistry and toxicology groups. She was a recipient of the Thieme Chemistry Journals Award in 2021.

INTERVIEW

SYNFORM *What is the focus of your current research activity?*

Prof. A. Voutchkova-Kostal As a graduate student in the later 2000's, I remember noticing that research in catalysis almost exclusively focused on selective bond construction. It was clear why: making molecules creates value, unlike breaking them down. I wondered what the value proposition of bond cleavage might be, and indeed, within the next few years, that question was answered. Research in valorization of biomass through selective bond cleavage exploded. As numerous new catalytic routes for breaking bonds in lignocellulose were developed, chemists looked towards the next challenge in breaking bonds of synthetic polymers, like plastics. I have been interested in selective defunctionalization of chemicals for many years now, and especially in how it can be applied to creating circular economies and cleaner syntheses. Among the current research efforts in our group that exemplify these goals are the depolymerization of lignocellulose PET using ionic liquids designed to have low ecotoxicity, and the use of decarbonylation and dehydrogenation chemistry to defunctionalize and couple substrates. When designing new processes, we assess whether it can deliver a quantifiable decrease in environmental impact over alternatives, and minimize the hazard of chemicals we are using and making.

SYNFORM *When did you get interested in synthesis?*

Prof. A. Voutchkova-Kostal I got interested in synthesis through cooking. I loved cooking and baking when I was young, and later got interested in formulations for making cosmetics. In high school and college I enjoyed learning about the chemistry of cooking and baking. I really enjoyed organic labs in college, probably because we had a really engaging instructor who made them fun. I decided to try out synthesis

in industry, and got an internship in a pharma company one summer. In those few months I realized that while I did love synthetic chemistry, I did not want to just follow prescribed procedures. In fact, I kept modifying the protocols I was given and trying new reactions, which probably frustrated my poor mentor! He recommended that I pursue graduate school to see if I had what it takes to do research. At Yale I got to take organometallic chemistry with John Hartwig, who was an incredible instructor, and the course really opened my eyes to the potential creativity of catalysis in designing new and more efficient reactions. I do my best to pass on that spark to my students in organometallics now.

SYNFORM *What do you think about the modern role and prospects of organic synthesis?*

Prof. A. Voutchkova-Kostal Nature creates an impressive spectrum of biological structures and functions from a small handful of elements, efficiently cycling every nutrient in making and re-making living things. Traditionally, organic synthesis has been focused on bond construction to access some of nature's structural diversity (e.g. natural product synthesis), but not much emphasis has been placed on design for breakdown, either biological or synthetic, and on design for minimal hazard. I think we are at the brink of a revolutionary phase in organic synthesis: if we, as synthetic chemists, embrace the challenge of designing molecules and clean synthetic routes to allow for circularity and intentional minimization of hazard, we will play a critical role in the transition to circular economies. This is a very exciting time to be an organic chemist, and an opportunity to recruit a new generation of environmentally conscious chemists to help make this vision a reality!

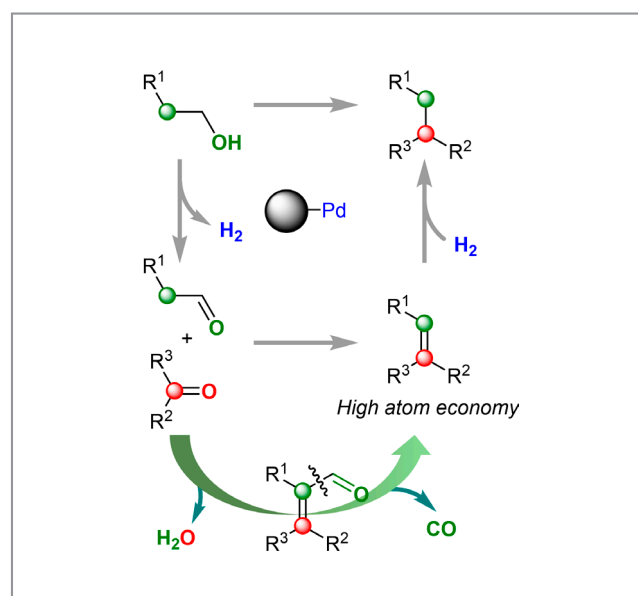
SYNFORM *Could you tell us more about your group's areas of research and your aims?*

Prof. A. Voutchkova-Kostal Our group focuses on design of chemical processes that involve defunctionalization reactions, such as dehydrogenation, decarbonylation, decarboxylation, transfer hydrogenation and hydrolysis, among others. These kinetically challenging reactions have been traditionally catalyzed by organometallic catalysts consisting of precious metals, which are typically not feasible on a large scale. Our interest therefore lies in developing relatively cheap and robust heterogeneous catalysts for these transformations that can work under mild conditions. This requires understanding how to "tune" the reactivity of these materials, which has led us to explore the electronic effect of supports on immobilized nano

species. Our most successful and versatile catalyst system consists of group 10 metals immobilized on tunable layered double hydroxide clays (hydrotalcites). We have shown that these materials have a number of advantageous properties that we can exploit by incorporating a second transition metal with synergistic activity. For example, we find that Cu-doped hydrotalcite is an excellent support for iridium-based single-site catalysts for transfer hydrogenation from glycerol to CO₂, making two valuable products: lactic acid and formic acid (we thank the NSF CAREER program for supporting this work). We have also shown that these catalysts have multiple catalytic sites that we can exploit for tandem transformations: a feature we are now exploiting in the defunctionalization of lignocellulose.

SYNFORM *What is your most important scientific achievement to date and why?*

Prof. A. Voutchkova-Kostal On the catalysis front, we are excited about expanding our work on multifunctional catalysts. For example, we designed a Pd-hydrotalcite catalyst that can facilitate decarbonylation, dehydrogenation and aldol condensation, which allows the conversion of alcohols into long-chain olefins (Scheme 1; *J. Am. Chem. Soc.* **2020**, *142*, 696–699; *ChemRxiv* **2021**, preprint, DOI: 10.26434/chemrxiv.14292311.v1). This chemistry can also be performed with



Scheme 1 Multicomponent catalytic system based on Pd-hydrotalcite heterogeneous catalyst, for the dehydrogenative and decarbonylative coupling of alcohols or aldehydes.

aldehydes, in which case it is an atom-economical analogue of a Wittig reaction. We have extended this chemistry recently to biomass-related substrates, such as lignin, allowing us to carry out multiple tandem reactions with just one catalyst. On the chemical design front, I am most proud of collaborative work on the development of in silico predictive tools for a number of toxicological endpoints, such as skin sensitization and aquatic toxicity. It has been extremely rewarding to see these tools used by industry to assess hazard of chemicals used in manufacturing. My colleagues and I hope this work helps protect human health, and hopefully also saves the lives of a few critters used in animal testing!

A handwritten signature in orange ink that reads "Matthew Farnok".