Catalysis and Sustainability – A Key Tool in Pharmaceutical Sciences: A Candidate's personal Journey of Innovation

Dr. Basker Sundararaju (BS) is a well-trained organometallic catalysis chemist and has been fervently dedicated to research in the general area of 3d-transition metal catalysis for organic synthesis. His interest and passion lie in developing novel catalytic systems that are sustainable, expand academic horizons, and offer transformative solutions to bioactive compounds and pharmaceuticals, besides his key contribution to energy storage materials, waste-recycling to society's most pressing challenges.

Catalysis with 3d-metals for direct hydrocarbon functionalization was in its infancy (*ACS Catal*. 2022, *122*, 3452) a decade ago. Unlike Noble metal catalysis, understanding the mechanistic intricacies of 3d-metal catalysis, which can proceed via one or two electrons and change their spin state depending on reaction conditions, is nontrivial. Hence, the early part of BS's independent career was devoted to systematically understanding the reactivity patterns of iron, cobalt, and manganese-based catalysts. In this regard, BS spearheaded advancements in C-H bond functionalization (*ACS Catal*, 2016, *6*, 2792, *Chem. Sci*. 2017, *8*, 2431, *ACS Catal*. 2018, *8*, 8115), late-stage derivatization of drugs and organic/organo-metallic materials, and the synthesis of chiral drug synthons and asymmetric molecular entities. He demonstrated the application of these catalytic systems for late-stage modifications of commercially available drugs such as Telmisartan, Gemfibrosil, Naproxen, and others (*Catal. Sci. Technol*. 2018, *8*, 5963), showcasing the practical utility and versatility of his methodologies in the pharmaceutical industry.

BS's systematic and focused efforts in understanding the chemistry of high-valent cobalt have culminated in the development of other catalytic processes, including hydrogenation (*ChemSusChem*, 2019, *12*, 3089), dehydrogenation chemistry (*ChemSusChem* 2019, *11*, 5160, *ACS Catal*. 2020, *10*, 8023, *ACS Catal* 2021, *11*, 11906, *J. Catal*. 2023, *88*, 5893), and chiral versions of cobalt-catalyzed systems (*Angewante Chemie Int. Ed*. 2024, *63*, e202315005, *Angewante Chemie Int. Ed*. 2024, in press). He also developed well-defined chiral Cp*Co(III) complexes for hydrogen evolution and oxygen evolution reactions (HERs and ORRs). Furthermore, his recent efforts on utilizing patented chiral Mn-based catalysts for asymmetric hydrogenation of various unsaturated substrates, leading to chiral amine, lactone, and chiral diol synthesis using molecular hydrogen as the sole reductant, are noteworthy (Indian Patent, 2024 submitted). Some of these processes are at TRL-3, and engagement with industry is expected to advance them to TRL-6/7.

A testament to his accomplishments is the development of novel Cp*Co(III) catalysts HER with a turnover frequency (TOF) close to 110,000 per second per site, a milestone in catalytic science (*Catal. Sci. Technol*. 2024, in press). This groundbreaking achievement has set a new benchmark for turnover frequency in homogeneous catalytic systems, offering a glimpse into a future powered by sustainable energy solutions. Furthermore, BS's team explored metallophotoredox catalysis under 3d-metal catalysis for for biomimetic synthesis of terpenol derivative starting from prenol to C40 carbons (*Nat. Commun*. 2024, in press). The outcomes of his ardent research

endeavours over a decade on 3d-metal catalysis have translated into several high-impact peer-reviewed journals, solidifying his status as an expert in the catalysis community.

Establishing himself as an active researcher in catalysis, BS has begun to work on problems of greater societal concern, such as polymer degradation (upcycling/recycling), CO_2 to fuels, and C1-based fine chemicals. Addressing the urgent need to tackle environmental non-degradable waste accumulation, BS has developed an approach to plastic waste recycling. He has produced an inexpensive cobalt catalyst that converts plastic waste (e.g., PC, PET, and PLA) into monomers along with methanol by hydrogenolysis. By grafting the catalyst onto a solid support, BS aims to develop a scalable recycling process for industrial applications, contributing to sustainable carbon neutrality. By harnessing the power of chemical hydrogenolysis, BS has unlocked the potential to convert polymer waste back into its monomeric forms, making an invaluable contribution to the circular economy, where waste is transformed into an opportunity.

Simultaneously, BS embarked on research of relevance to battery technology through the development of novel 2D organic materials. His recent work on ionic covalent organic frameworks has redefined the boundaries of energy storage, boasting charging and discharging efficiencies tenfold higher than conventional polymer-based electrolytes (*Indian patent* 2024 submitted). With a provisional patent filed, BS eagerly anticipates this contribution in battery technology to translate into a product, exemplifying a case of academic curiosity translating into technology transfer for societal needs.

One of his relentless pursuits is the conversion of CO_2 into diesel fuel. Leveraging metal-free carbonaceous 2D networks as heterogeneous catalysts, he has made headway in the effective capture and conversion of CO_2 into a viable energy source (*Indian patent* 2024,submitted). With a reversible catalytic system promising to revolutionize industrial processes, BS is on the cusp of developing a candidate for CO_2 conversion, which may constitute a significant contribution to sustainability.

In summary, BS is a dedicated scientist par excellence. As a highly committed scientist with relentless pursuits in research geared towards solutions for humankind's pressing challenges, BS has carved a niche for himself globally in the development of earth-abundant Co-based catalysts. His key contributions on asymmetric catalysis directly by activating carbon-hydrogen bond, and this emerging and ever expanding field have a huge impact on the pharmaceutical industry.

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Basker Sundararaju

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