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Development of Sustainable Organocatalytic and Photocatalytic Methods for Selective Carbon–Carbon and Carbon–Heteroatom Bond Formation

DR. K. S. LAMANI
Associate professor, Department of chemistry, C.S. Bembalagi, S.M.R.Palaredha science and G.L.Rathi commerce college Ramdurg

Abstract- ***In organic synthesis, one of the primary goals remains the creation of carbon-carbon and carbon-heteroatom bonds due to the fact that these bonds form the framework and diversity essential for pharmaceuticals, agrochemicals, natural products, polymers and advanced functional materials where carbon-nitrogen, carbon-oxygen, carbon-sulfur and carbon-phosphorus bonds play significant roles in controlled molecular recognition, reactivity, biology activity and material performance. Conventional methods of forming such bonds may require stoichiometric conditions, harmful solvents, extensive energies, few rare or toxic metals and low yield reactions or generate a significant amount of side-products, which leads to practical difficulties and concerns regard to purification, green chemistry and selection (Anastas & Warner, 1998; Sheldon, 2017). In contrast, the complementary methods of organocatalysis and photocatalysis has come into being to circumvent such drawbacks that can be achieved through the assistance of organocatalysts or light energy. On the one hand, organic catalysts act through Brnsted acids/bases catalysis or N-heterocyclic carbene catalysis, via enamine/iminium activation and hydrogen-bond activation or other activation modes of organic catalyst. On the other hand, photocatalysts mediate reactions by light through the excited state and reactive species or electron transfer process at relatively gentle conditions (Dalko & Moisan, 2004; Melchiorre, 2018). Therefore, herein we present a conceptual sustainable model framework, combining organic catalysis, photocatalysis, hydrogen-bond catalysis, enamine/iminium activation, N-heterocyclic carbene catalysis, radical mediated bond formation strategy and selected reaction mediums together with optimized strategies including minimizing solvent utilization and energy inputs, together with computation, mechanics research and green chemistry metrics as additional tools. Emphasis is particularly placed on designing highly effective catalysis that ensures high conversion, yield, chemo selectivity, regioselectivity, enantioselectivity, while minimum the loading of catalyst, generated hazardous waste, depended of metals and non-necessary chemical synthesis steps/operations. Contribution aims at creating a conceptual methodology toward selective C-C and C-heteroatom bond constructions by molecular catalysis and visible light mediation with sustain process design that is expected to benefit organic synthesis and pharmaceuticals, agrochemicals, natural-product and materials science fields. However, all the proposed models must be critically examined via mechanistic studies, lifecycle analysis, experiments tests etc before any claims regarding to their industrial sustain can be warranted.***

Keywords: Organocatalysis; Photocatalysis; Carbon–carbon bond formation; Carbon–heteroatom bond formation; Green chemistry; Visible-light synthesis; Sustainable organic synthesis; Asymmetric catalysis

I. INTRODUCTION AND BACKGROUND RELATED TO THE STUDY

Selective formation of chemical bonds is paramount in organic synthesis because controllable formation of the C–C, C–N, C–O, C–S, and C–P bonds generates molecular connectivity necessary to build the structural complexity, stereochemistry, and functional properties essential in drugs, agrochemicals, natural products, polymers, dyes, and electronic materials, and other value-added chemicals, whereas ability to construct such bonds selectively directs an efficiency, safety, and practicability of a multistep sequence. Traditional strategies to synthetic chemistry typically relied on vast usage of transition metal catalysis, stoichiometric coupling or activating agents, strongly oxidizing or reducing agents, high-temperature processes, and protection-group chemistry, offering a number of valuable transformations, but it often results in extra steps, an amount of solvents, an extra of purification, an excessive waste produced, as well as potential danger derived from either use of residual metals, either toxic reagents (Anastas & Warner, 1998; Sheldon, 2017); although transition metal-catalysis are

extremely efficient toward selective bond formation, metal atoms such as Pd, Pt, Rh, Ir are not resource rich, which often concern resources limitations, cost-performance, and residual metals that needs removal, if high purity products are demanded. Using stoichiometric reagents in couple with protected compounds gives rise to loss of atoms, owing to auxiliary molecules or unnecessary operations which contribute nothing toward final target structure. So does applying strongly oxidizing/reducing agents and high-temperature processes consuming too much of energy, leading to unwanted byproducts and making it essential to invent such organic transformations that achieve atom economy. These shortcomings has made efforts towards sustainable catalysis to be further pursued, that aims at merging synthetic efficacy with ecological responsibility; thus sustainable alternatives to synthetic procedures as different from traditional one, such as organocatalysis, photocatalysis, photoredox reaction, one-pot reaction, and renewable feedstock-based synthesis have been introduced. The organocatalysis involves a variety of organic small molecules that transform substrates through enamine formation/iminium activation mechanism, hydrogen-bonding effects, Brønsted acid/base activation, N-heterocyclic carbene catalysis etc., offering an alternative tool for both metal-containing and metal-free bond formation, many of which are enantioselective transformations (Dalko & Moisan, 2004; MacMillan, 2008); photocatalysis and photoredox activation exploit captured light to reach electronically excited states thereby yielding electronically excited species for reaction through either an energy- or photo-electron transfer (PET) reaction, often under fairly mild conditions, an enormous amount of literature works on various radical mediated C-C and C-heteroatom bond constructions via photoredox organic catalysts has recently become available (Romero & Nicewicz, 2016). Moreover, one-pot or two-pot or telescoping strategy avoids isolation of intermediate, which can efficiently decrease use of solvents, of purification, and time, and solvent-free or low-solvent strategy, also decreases quantity of volatile organic compounds produced as well as physical matter flow; on another hand, the organic resources such as renewable feedstocks are considered a sustainable alternatives to some fossil carbons in producing valuable organic molecules. Therefore, the combination of organocatalysis, photoredox mechanism with catalysis from light, atom-effective reactions and strategies of reaction design/engineers, renewable resources, green chemistry principles has provided a conceivable framework to pursue the selective chemical bond formation via higher synthetic yield with less environmental impact.

II. HISTORICAL DEVELOPMENT

Historically, sustainable organocatalytic and photocatalytic chemistry has seen a progression from enzyme mimic and nature inspired catalytic systems to sophisticated small molecule catalysts and light induced reactions: Early on, chiral organic catalysts, in the guise of cinchona alkaloids, were shown to catalyze asymmetrical transformations; later, it was recognized that amino acids themselves and their derivatives are capable of effective catalytic activation; Hajos-Parrish and related proline catalyzed intramolecular aldol reactions and similar reactions of the 1970's can be seen as a foundation in amino acid catalysis, which later was augmented by both the independent work of List, Lerner, and Barbas and MacMillan on intermolecular proline catalyzed aldol reactions and imidazolidinone catalyzed asymmetrical Diels-Alder reactions, respectively, in 2000, bringing modern organocatalysis into fruition (List et al., 2000; Ahrendt et al., 2000; MacMillan, 2008); subsequently, organocatalysts developed from proline derivatives and sec.-amines to thioureas and other hydrogen bond donors, Brønsted acids-chiral phosphoric acids-were introduced and catalysis mediated by them under circumstances where Brønsted-acid activation is required to form reactive intermediates; introduction of NHCs followed, which through generation of active acyanionic intermediates were capable to catalyze C-C and C-heteroatom bond forming reactions (Dalko & Moisan, 2004; Enders et al., 2007); in parallel, photochemical catalysis evolved from standard photochemical activation of molecules and excited sensitisers that transfer energy or electrons to molecules in some way toward visibility-light photocatalysis / modern photoredox catalysis wherein activated photo-catalysts could be seen to facilitate the photoinduced electron or energy transfer; organic photoredox catalysts, including organically synthesized organic dyes, related chromophores etc. Were introduced which are useful, organocatalysts

without metals (Romero & Nicewicz, 2016). A particular advance in subsequent years was the convergence of these fields. Through their combination enamine, iminium, Brønsted acid/base and NHC catalysis can be combined to processes difficult to access through both mode or another only; asymmetric photoreactions have come to their prime, stereo chemically controlled by either organocatalysts or other species while light induced processes generate/activate species facilitating the reaction (Zou et al., 2018; Proctor et al., 2018). Now, February 2025, convergence has matured to form a wide area encompassing dual and cooperative catalysts organic photoredox catalysts radical-mediated stereoselective synthesis and a bifunctional chiral photocatalytic system, demonstrating the journey starting from enzyme mimic reaction, via catalysis by organocatalysts into the area of visible-light photoreactions.

III. RESEARCH PROBLEM

High bond formation efficiency and perfect selectivity within low environmental, consumption and implementational limits while maintaining the chemical transformation itself remains one of the key challenge in current catalytic organic synthesis, since it involves hazardous reagents, hazardous or persistent solvents, stoichiometric activating reagents and activating agents or energy consuming conditions-resulting in generation of hazardous or persistent species, risk upon toxicity, presence of toxic metallic residues, high demands for purifications and in essence unsustainable process (Anastas & Warner, 1998; Sheldon, 2017). The development of catalytic asymmetric methodologies based on transition metals made it possible to get perfect selectivities on C-C as well as C-heteroatom coupling, however the scarcity and price related concerns and presence of residual metals often raise issues over their usability in the pharmaceutical and fine chemical industries whereas low atom economy, stoichiometric amounts of byproducts will necessarily involve a huge impact upon material and environment. Measures like Atom economy, E-factor and Process mass Intensity (PMI) have already become standard criteria to realize, whether any modification does bring improvements or not, and there are always associated factors to consider including solvent usage, process life cycle, etc (Sheldon, 2017). Organocatalysts, which substitute for metal catalysts, have resolved some of the above cited issues, but suffer from issues like the requirement of high loadings of catalyst and wide variations of catalyst loading among different reactions and different transformations, sensitivity of the reactions to reaction condition, problems concerning retrieval and reuse, narrow substrate scope, while lacking any kind of validation at higher scale. Similarly, the photocatalysts fulfill many of these green chemistry concerns, but they have certain drawbacks such as poor yields with low loading of catalyst for most reactions. The development in photocatalytic reactions have issues in process translation such as penetration of light in reactor, utilization of photons as well as heat management of the system, reactor design as well as mass transfer efficiency changes drastically once you go from lab-scale (mg to gram level) to pilot-plant and large-scale plant level-so reactor engineering, concept of continuous-flow technology etc are key at these stages (Zondag et al., 2023). Thus, it should not just involve substitution of metal catalysts with organic catalysts or instead of conventional heating to irradiation. Rather we aim for integrated catalytic architecture where molecular design, substrate activation, mechanism, catalyst stability and reactor engineering should work simultaneously for high conversion, yield, perfect selectivity (chemo, regioc and enantio), low catalyst loading, waste generation, solvent usage and low energy consumption. Green chemistry tools need to focus on development of efficient, selective and recyclable catalysts for C-C and C-heteroatom coupling reaction. The catalyst must ultimately contribute positively to selectivity, recyclability, environmental suitability and scale of reactions and proposed improvements of synthesis must be proven by valid quantitative green parameters & experimental validation

IV. LITERATURE REVIEW

There are a range of complementary methods that can be used to effect catalytically ‘active’ or ‘activated’ organocatalysis. These utilize a small organic molecule to promote reactivity and control pathway specificity for a broad variety of C-C and C-heteroatom bond formation reactions. Secondary amines, particularly proline derivatives, are a cornerstone of organocatalysis because they reversibly

react with a carbonyl partner to form enamines, which function as nucleophilic intermediates for functionalization chemistry and stereoselective reactions like aldol, Mannich, and Michael addition. Enamine catalysis cycle involves: formation of the enamine; reaction with an electrophilic partner; hydrolysis; and amine catalyst regeneration (List et al., 2000; Mukherjee et al., 2007). In contrast, activation of electrophilic reaction partners using chiral secondary amines generates iminium ions which are transient electrophiles that decrease the activation energy of nucleophilic addition. This strategy of iminium catalysis has unlocked important conjugate addition, cycloaddition and functionalization of carbonyl-derived substrates, and it is very useful in asymmetric synthesis through stereo controlled spatial environments induced by chiral amine scaffolds (MacMillan, 2008). Hydrogen-bond catalysis with a hydrogen-bond donor motif-thioureas, squaramide's, and urea derivatives, for example-is another important non-covalent method for activating substrates through substrate organization, stabilizing charge distribution within the transition state, increasing rates, and improving reaction rates and selectivity. In a more advanced scenario, chiral bifunctional catalysts can provide simultaneous activation of nucleophile and electrophile partners (Doyle & Jacobsen, 2007). A prominent form of Brønsted acid organocatalysis, exemplified by chiral phosphoric acid catalyzed reactions involving catalysts derived from BINOL-type scaffolds, plays a significant role in contemporary synthetic efforts.

Here, protonation of nucleophile and stabilization of intermediates through a combination of proton transfer, and chiral phosphate mediated hydrogen bonding provides activation of electrophiles and enforces stereochemical control to influence selectivity for a plethora of new carbon-carbon and carbon-heteroatom bonds via addition, cycloaddition, rearrangement and asymmetric dearomatization processes (Akiyama, 2007; Terada, 2009). Catalysis with N-heterocyclic carbenes (NHCs) utilizes an 'umpolung' mechanism in which nucleophilic carbene reacts with carbonyls leading to the formation of Breslow type intermediates which can then function as acyl anions or their equivalents, thereby unlocking key benzoin, Stetter, annulation, and a host of other C-C and C-heteroatom coupling reactions. Developments through February 2025 further confirm that NHC chemistry also encompasses radical and photoredox strategies demonstrating the wide breadth of mechanisms and reactivity being discovered in this area of organocatalysis (Enders et al., 2007; Flanigan et al., 2015).

V. RESEARCH METHODOLOGY

The presented catalytic selection process for novel organocatalytic and photocatalytic systems is established on a rational assessment scheme and intends to pinpoint catalytic structures to provide effective, selective, and "green" C-C and C-heteroatom bond formations where individual candidates have to be chosen on the basis of multiple correlated parameters such as catalytic activity, selectivity, toxicity, chemical stability, synthetic accessibility, recyclability, and the green chemical impact where higher catalytic activity should be an indispensable attribute as effective catalyst promote substrate activation, boost reaction rate and facilitate high conversion under moderate conditions also decreases its requirement. And then, evaluate the selection process for ability of catalytic system architectures to control over the chemo selectivity, regioselectivity, as well as enantioselectivity through precise geometrical influence to the intermediate and active complexes in reaction path and regulating the mechanism (MacMillan, 2008). Also, the low toxicity and low environmental impact should be fundamental issues when designing catalytic systems due to minimize the hazard material, non-polluted compounds and waste as well as conform to green chemistry notion (Anastas & Warner, 1998) and then, catalytic systems with greater stability is necessary and vital because the reliability of catalyst in sustained applications and the possible catalyst deterioration have influenced the efficiency and durability; it is desirable and economical to develop easily accessible and synthetic rout in the development of catalysts as well as high recovery and recycle of catalysts to improve the efficiency and reduce the amount of waste, where recycle of the catalysts play crucial role in sustainability evaluation criterion. Additionally, the simulation approach including the calculation on molecular modeling, density functional theory, or date-oriented catalyst designing might assist the evaluation before experiments with estimating the

structural characteristics of catalyst and the potential catalytic activity and selectivity as well as activation barriers and transition state (Tropsha, 2010). Eventually, in such presented conception and methodology, based on the principles of molecular design, mechanistic consideration, numerical calculation, and green chemical concepts, it has offered a guideline toward exploring design and choice of upcoming organic catalysts and photocatalysts of which high performances combined with high sustainability and potential for the advance chemical transformation.

VI. COMPUTATIONAL CATALYST DESIGN

Computational catalyst design is the indispensable complement to contemporary sustainable organic synthesis, since it generates methods for the prediction of catalyst performance, structure optimization, and the rapid exploration of effective catalyst systems that promote selective formation of both C–C and C–heteroatom bonds. Catalysis-substrate interactions, conformation preferences of a given catalyst and potential reactive pathways are computationally accessible via investigations of how molecular properties affect activation of the substrate, organization of transition states, and selection of desired products using molecular modelling techniques. They also help to select promising catalyst scaffolds prior to empirical tests. Conformational considerations have proven critically important in enantioselective reactions because stereochemical events and efficiency depend on miniscule changes in catalyst topology, steric interactions and non-bonding effects (Cramer, 2004). Density Functional Theory (DFT) has been established as an efficient approach towards investigating catalyst performance, providing energetic analysis including energy barriers and the stability of intermediates; molecular orbital theory and descriptions of electron transfer were developed for the organo- or photocatalytic cycle of reactions that proceeded through hydrogen bonding, radicals, charge-transfer (CT) event or excited-state reaction mechanism (Parr & Yang, 1989). DFT calculations also help with competing mechanistic analysis and to provide justification of empirical trends of selectivities in reduced needless experimental work; machine learning/AI techniques could also advance catalyst design on data of chemical sets and molecular descriptors of reaction data to predict reaction pathways, screening catalysts, optimizing parameters or generating retrosynthetic strategy or predicted yields. The conceptual framework illustrates an integrated approach for developing sustainable organocatalytic and photocatalytic systems by combining rational catalyst design, computational prediction, mechanistic understanding, and green chemistry principles, where organic catalysts such as proline derivatives, chiral phosphoric acids, thioureas, squaramides, and N-heterocyclic carbenes are designed to promote selective substrate activation through enamine, iminium, hydrogen-bonding, Brønsted acid, and umpolung catalytic pathways, while photocatalytic systems utilize visible-light activation to generate excited states, electron-transfer processes, and reactive intermediates for efficient bond construction; molecular modelling and density functional theory calculations provide insight into catalyst–substrate interactions, conformational behaviour, activation barriers, transition states, and reaction mechanisms, whereas machine-learning approaches support catalyst screening, reaction prediction, and optimization of synthetic conditions; this integrated methodology aims to achieve selective carbon–carbon and carbon–heteroatom bond formation with improved conversion, selectivity, reduced waste generation, lower energy consumption, minimized toxicity, and enhanced sustainability, thereby establishing a future-oriented platform for efficient organic synthesis in pharmaceutical, materials, and industrial chemistry.

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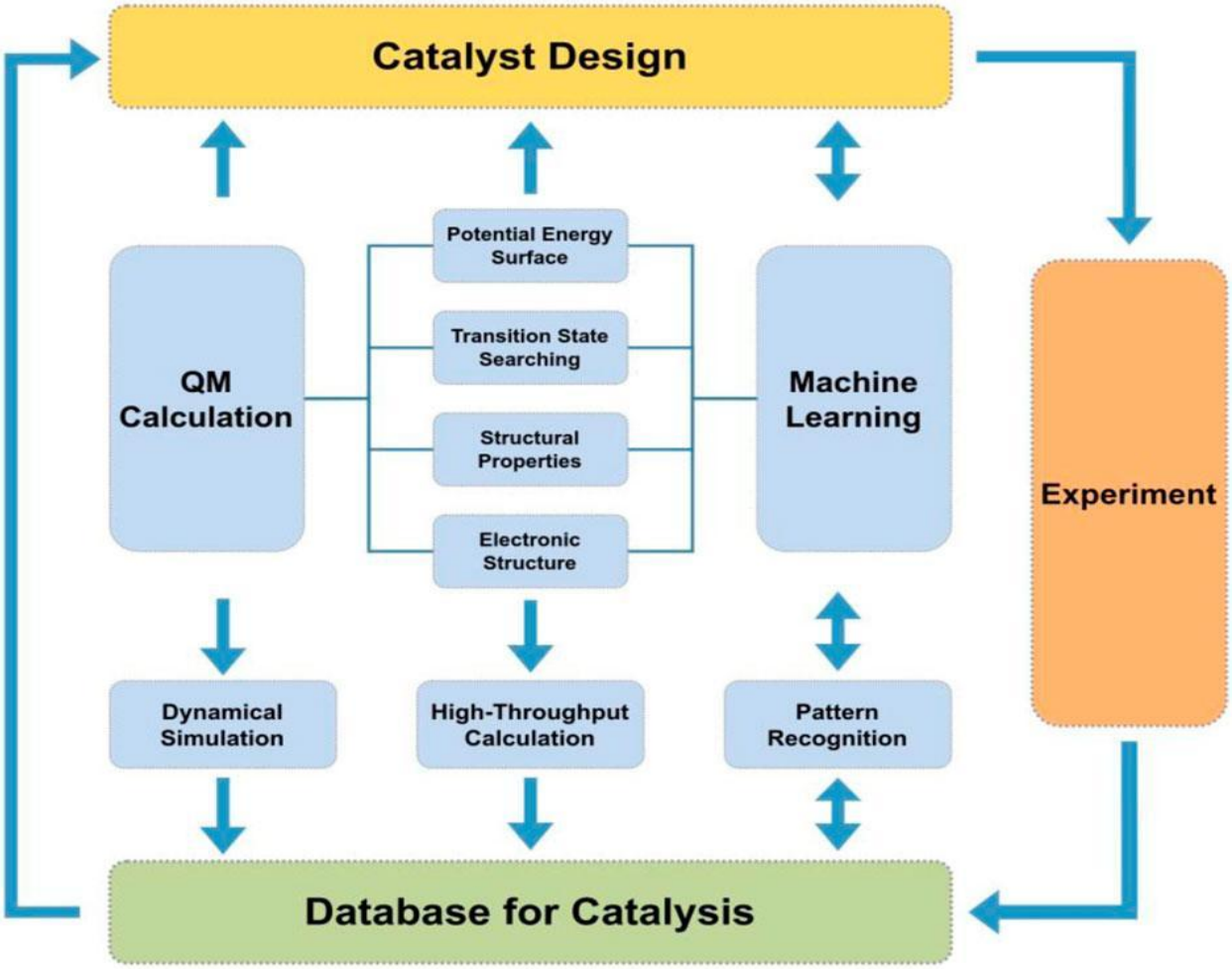

Above diagram showing Development of Sustainable Organocatalytic and Photocatalytic Methods for Selective Carbon–Carbon and Carbon

VII. DISCUSSION

The development of sustainable organocatalytic and photocatalytic processes offers an avenue to dramatically enhance the capabilities of modern organic synthesis through the creation of efficient, selective, environmentally sound transformations by meticulously controlling aspects of catalyst structure, mechanism and substrate activation which is explained in more detail with higher efficiency by being achieved through better molecular optimization, greater stability of transient intermediates, more effective reaction paths all to lead higher substrate conversion, higher product yield and more reduced catalyst loading than can be expected with current catalyzed reactions thereby both economic value and practicality are increased (MacMillan, 2008), higher selectivity with chemistries predicted through rational catalyst design with influence upon molecular recognition, transition state organization and reaction path such that control is exerted upon not only chemical reaction taking place, but at what position as chemoselectivity (preferring the functional-group-dependent reaction pathway and ruling out side reactions), regioselectivity (where it would ideally be preferred that bond formation occur), and importantly enantioselectivity through stereo chemically pure catalytic systems such as stereo chemically pure proline, phosphoric acid etc catalysts etc. (List, 2007) with reduced waste, reduced solvent usage, reduce energy usage with milder conditions and visible-light or controlled activation and reduced reliance upon less desirable transition metals in the pursuit for sustainable methods that work for everyone (Anastas & Warner, 1998; Sheldon, 2017) Structure-Activity Relationship This is essentially the guiding factor

determining how effective a catalysis performed is with an organocatalysts or photocatalyst whereby catalyst structure dictates molecular interactions with the substrate, which dictates how active the pathways may or may not be. Factors which determine this are hydrogen-bonding capability, relative size and conformation of bulky substituents, electronic nature etc. Modifications at these sites are where optimization would occur for catalysis performance with computational models aiding investigation of mechanisms where experimental verification has played and will continue to play a crucial role along with mechanistic insight into where catalyst properties could be altered to drive reactions more effectively; this coupled with the principles stated above toward next-gen orgno and photo catalysts of high efficiency and excellent selectivity with low environmental toll

VIII. APPLICATIONS

Both sustainable organocatalytic and photocatalytic methods are widely applicable to a large range of problems within the context of pharmaceutical chemistry, the synthesis of natural products, agrochemical development and materials science due to their inherent ability to deliver control over carbon-carbon and carbon-heteroatom bond formation, thus enabling the synthesis of complicated architectures with precise stereo control, fine tuning of functionality and a high degree of control over the potential activity profile. Within pharmaceuticals, organocatalytic and photocatalytic transformations play a vital role, offering a number of strategies with significant advantages in the synthesis of pharmaceutically active agents and advanced intermediates due to their utility in selective transformations, stereospecific bonds and, critically, late-stage functionalization: the latter allows modification of biologically active molecules in advanced synthetic steps with minimal rebuilding of molecular architecture. This is advantageous as it permits improved efficiency and facilitates the design of novel drug candidates (MacMillan, 2008). Chirality, though, is pivotal to the biological selectivity, absorption, metabolism and overall pharmacological activity and hence its precise control, often through asymmetric organocatalytic procedures forming chiral intermediates, is essential in any modern drug discovery programme. With regard to natural products, both organocatalytic and photocatalytic transformations offers a way to construct structurally diverse molecules featuring several stereocenters and a variety of functional groups. Both systems promote efficient carbon-carbon bond formation, the construction of complex ring systems and late-stage functionalization allowing these transformations to produce such complicated natural products efficiently (List, 2007). It is in the realm of agrochemicals that organocatalytic and photocatalytic catalysis may lead to the formation of precise and environmentally friendly agrochemicals due to enhanced selectivity, reduced waste and the implementation of 'green' chemistry principles rather than using hazardous reagents; this may potentially streamline manufacturing procedures. In materials chemistry, organic molecules, monomeric intermediates to advanced polymers and conjugated systems may be selectively created, the precise control offered enabling fine tuning of optoelectrical and mechanical properties and as such facilitating the development of materials for use within organic semiconductors and various energy related technologies. Consequently, both organocatalytic and photocatalytic processes applied on a molecular design level offers a flexible solution for the manufacturing of important organic species for diverse industries, while also improving efficiency and enhancing "green" chemistry aspects.

IX. SIGNIFICANCE OF THE STUDY

The implications of developing new sustainable organocatalytic and photocatalytic approaches toward the construction of chemo-, regi-, and stereoselective C–C and C–heteroatom bonds are of relevance in science, environmental issues, pharmacy, and industry for the reason that such new catalytic strategies will open a door to controlling molecule construction, increasing efficiency, high selectivity and environmental benefits; from a scientific point of view, this field is an extension of organocatalysis through an in-depth exploration of small organic molecules as highly efficient catalysts to facilitate substrate activations via hydrogen-bonding, covalent catalysis, Brnsted acid/base mediation, and enamine, iminium and N-heterocyclic carbene catalyzed processes, while to that of photocatalysis via the use of light and radicals as key activating components to access transformations for bond constructions based

on visible-light-enabled reaction cascades, radical generation, and photoredox catalysis, MacMillan, D.B. (2008); Romero, N.A. Nicewicz, D.A. (2016), contributing to a better understanding of catalysis mechanism based on structure of interaction and transition-state effect, as well as the chemo-/regio-/enantioselectivity controlling of resulting product; while on the other hand, such sustainable catalytic systems address a range of environmental concerns including the reduction of hazardous reagent use and waste generation, the less consumption of organic solvent, lower energy requirement due to low reaction temperature, as well as the mitigation of environmental problems caused by toxicity, shortage and environmental contamination triggered by metal catalyst, Anastas P. T. Warner JC. (1998), Sheldon RA, (2017); The pharmaceutical importance is focused on an efficient construction for complex molecules and bioactive compounds and chiral building blocks needed in modern drug design, whose stereoselectivity and late stage modification will boost the advancement of drug discovery; On industrial scale it is possible to facilitate the bulk synthesis through improved catalytic efficacy of reaction, high simplicity of product isolation as well as the cost benefit of lower waste treating and higher economic efficiency, provided its stability, recoverability and feasibility as a whole are sufficient in large scale process; Thus, we anticipate that, together with computation chemistry design and green chemistry tenet, both organocatalysis and photocatalysis systems, can turn into successful candidates for the next generation of chemical technology with molecular accuracy, low impact of environment and commercial viability.

X. CONCLUSION

Organocatalysis and photocatalysis combined with other techniques offers promising tools for developing novel and practical protocols for sustainable organic synthesis which allows highly selective carbon-carbon and carbon-heteroatom bonds to be created through environmentally and economically viable, mild and catalytic manners in which organocatalysts precisely activate molecules through both covalently and non-covalently interactions while the photocatalytic systems employ light-mediated electron or energy transfer mechanisms to generate photoinduced species at milder reaction conditions; combined effects not only afford greater control of reaction stereoselectivity, reactivity, and molecular complexity, but more importantly minimize the reliance on reagents such as precious metal-catalyzed oxidants/reductants, excess solvent, extreme temperatures, and hazardous materials (MacMillan, 2008; Romero & Nicewicz, 2016) so as to achieve this; a suitable framework for the design of efficient new generation catalytic technologies capable of selective bond construction for environmentally friendly and highly effective organic synthesis consists of synergistic approaches namely molecular-driven catalyst design, rational mechanistic examination, theoretical calculations of catalysts as well as photocatalytic species as well as a comprehensive evaluation of green metrics. Computer simulations including molecular modeling, computational method on the basis of density functional theory, or artificial intelligence-aided prediction of catalysts may contribute significantly to this field and promote discovery from structural features of catalytic molecule to desired catalytic activity, which makes assessment of the ecological impact more robust by use of green metrics. Consequently, continuously developing green catalytic system with integrating organocatalysis and photocatalysis should pave the way for a future revolution of chemical manufacture characterized with high precision of synthesis, environmental benignancy and improved atom-, resource-, energy- and economy- efficiency, benefiting the pharmaceutical, materials and industry science application.

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