Smart Catalyst Design: Integrating Structure–Activity Relationships with Computational and Data-Driven Approaches

Ramandeep Singh[1], Rekha Rana[2], Subhi Sharma[3], Jeewanjot Singh[4], Isha dhiman[5] .Sahibpreet Singh[6] Aubair Manzoor Wani[7]

Assistant professor[1], Associate professor [2], Assistant professor[3], Assistant professor[4], Assistant professor[5] , UG Student[6], UG Student[7]

School of pharmacy, Desh Bhagat University, Mandi Gobindgarh, Punjab

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Abstract

Similar rational design of catalysts is a paradigm shift of the old-fashioned trial and error discovery to the predictive mechanism-oriented development of catalytic systems with improved activity, selectivity and stability. This review article reviews the current state of catalyst design in many related aspects: active site engineering, at both the atomic and molecular scale, improved structure-activity relationship (SAR) studies through operando characterization methods, computational and machine learning methods of catalyst screening and optimization, and creating sustainable catalytic processes, with respect to the principles of green chemistry. We critically examine recent advances in single-atom catalysts (SACs), metal-organic frameworks (MOFs), defect-engineered materials, and bifunctional catalytic systems and how interdisciplinary integration of chemistry, materials science, and chemical engineering has spurred this development. Special attention is given to the emerging approaches based on the exploitation of designer-like methods, high-throughput experimentation, and data-driven approaches, to explore huge compositional and structural spaces. The review is concluded with a prospective outlook of the persisting challenges and opportunities such as catalyst design of electrochemical reduction of CO2, biomass valorization, and ambient-condition fixation of nitrogen.

Keywords catalyst design, structure-activity relationships, single-atom catalysts, computational catalysis, active site engineering, green catalysis, machine learning, operando characterization

1. Introduction

Catalysis in the Middle of the Influence of Modern Society: In all of chemical manufacturing, nearly 90 percent of the processes are catalysed, and over 35 percent of gross domestic product (GDP) in the world is catalysed [1,2]. Catalysts are used in the transformation of petroleum into oil refining and polymer into plastics, pharmaceutical manufacturing and environmental cleanup, among others, where chemical reactions in either a kinetically or thermodynamically unfavorable manner would not otherwise be feasible. It is the Haber-Bosch process necessary to produce ammonia using iron-based heterogeneous catalysts that support approximately half of the global food production via the production of fertilisers alone [3]. With the society facing the mounting pressures in energy security, mitigation of climate change, and sustainability of resources, more efficient, selective, and durable catalytic systems are more than ever needed.

Empirical Discovery to Rational Design: Traditional catalyst development has been based traditionally on empirically-based methods of catalyst development (systematic screening of materials and reaction conditions through chemical intuition and experience). Although this paradigm has produced many commercially viable catalysts, it is inefficient in nature, as well as fails to harness the full potential of catalytic materials. The development of rational catalyst design is a radical shift in approach, in which the underlying knowledge in reaction mechanism, electronic structure, surface chemistry, and transport processes are used to predict and design catalytic behaviour in advance [4,5].

This change has been facilitated by a number of convergent developments: Atomic-resolution characterization techniques, such as aberration-corrected scanning transmission electron microscopy (AC-STEM), X-ray absorption spectroscopy (XAS) and scanning tunnelling microscopy (STM), that give the unprecedented understanding of catalyst structure at the atomic level [6]. Operando and in situ spectroscopies that enable one to study catalysts in working conditions, revealing transient intermediates and dynamic structural evolution [7]. Density functional theory (DFT) and more, which makes quantum mechanical predictions of adsorption energies, activation barriers, and reaction pathways on catalytic surfaces possible [8]. Machine learning (ML) and artificial intelligence (AI), which makes a rapid screening of large space of catalytic parameters and discovery of non-obvious structure-property correlations possible [9]. Highly versatile synthesis techniques such as atomic layer deposition (ALD), synthesis of colloidal nanocrystals, and self-assembly of metal-organic frameworks (MOFs) [10] provide a high level of control over the composition, morphology and structure of catalysts.

2. Active Engineering of Remarkable Catalysis

2.1 Single-Atom Catalysts (SACs)

2.1.1 Concept and Advantages

The smallest possible size of a catalyst is single-atom catalysts, where isolated metal atoms are spread over a support medium [11,12]. The field has experienced phenomenal growth since the seminal report by Qiao et al. in 2011 who showed that single Pt atoms on iron oxide (Pt1/Fe2O3) had superior CO oxidation activity [13]. SACs have a number of inherent benefits. They provide optimal efficiency in the utilisation as all metal atoms

are potentially catalytically active, and this is especially important in precious metals, including Pt, Pd, Ir, and Ru. The electronic structure of individual atoms of metals compares significantly to nanoparticles or bulk metals as a result of quantum confinement, charge transfer with the support, and unique coordination conditions [14]. Active sites are uniform in ideal SACs making it easy to study them mechanistically and provide a direct comparison with computational models. Structure-sensitive side reactions are usually suppressed by the presence of ensemble sites, and become more selective [15].

2.1.2 Strategies to Synthesize and Stabilize.

The major problem in the preparation of SAC is how to avoid aggregation of isolated metal atoms into clusters or nanoparticles in the course of synthesis and under reaction conditions. A number of strategies have been worked out to handle this difficulty:

a) Defect based anchoring and spatial confinement: Oxide, nitride and carbon surfaces have strong anchoring sites on their surface. An example of cation vacancies on CeO2(111) surfaces is that single Pt atoms can be trapped by strong metal-support interactions (SMSI), which has a binding energy of over 3 eV according to DFT calculations [16]. Likewise, utilising nitrogen-doped carbon materials (M-N-C) providing coordinatively unsaturated nitrogen sites that form stable M-Nx moieties, which have been studied broadly with Fe, Co, Ni, and Cu as single atoms in electrocatalysis [17]. Spatial confinement is achieved using Microporous and mesoporous materials, such as zeolites, MOFs, and covalent organic frameworks (COFs), may confine the atoms of metals in cavities or channels of a specific size. These hosts have steric constraints that block the migration and sintering of the metals. Single Rh atoms that are confined by zeolites have also shown an extraordinary stability and selectivity in the ethylene hydroformylation [18].

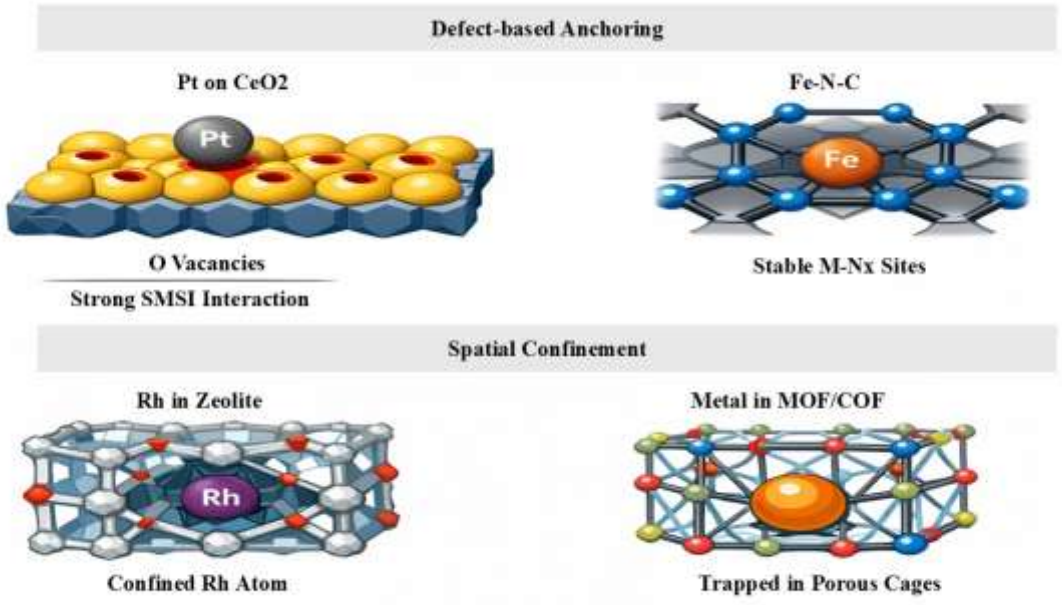


Fig.1 Defect-based anchoring keeps single atoms stable by using vacancies and interactions between metal and support. Spatial confinement keeps atoms from clumping together by trapping them in porous frameworks.

b) Supported strong covalent/ionic bonding and coordination engineering through wet-chemical means: Metal atoms may also be strongly bonded with support atoms, especially on reducible oxides (TiO2, CeO2, Fe2O3) and two-dimensional (2D) materials (MoS2, h-BN, graphene). The character of these interactions, i.e., ionic (e.g. Pt2+ on CeO2) or covalent (e.g. Pt on N-doped graphene) has a drastic impact on the electrical properties or catalytic characteristics of the anchoring atom [19]. Also, coordination engineering through wet-chemical routes facilitates stabilization of single metal atoms via tailored ligand design during synthesis. For instance, thiolate stabilized gold materials can serve as precursors that generate isolated Au atoms on different supports upon controlled thermal treatment [20].

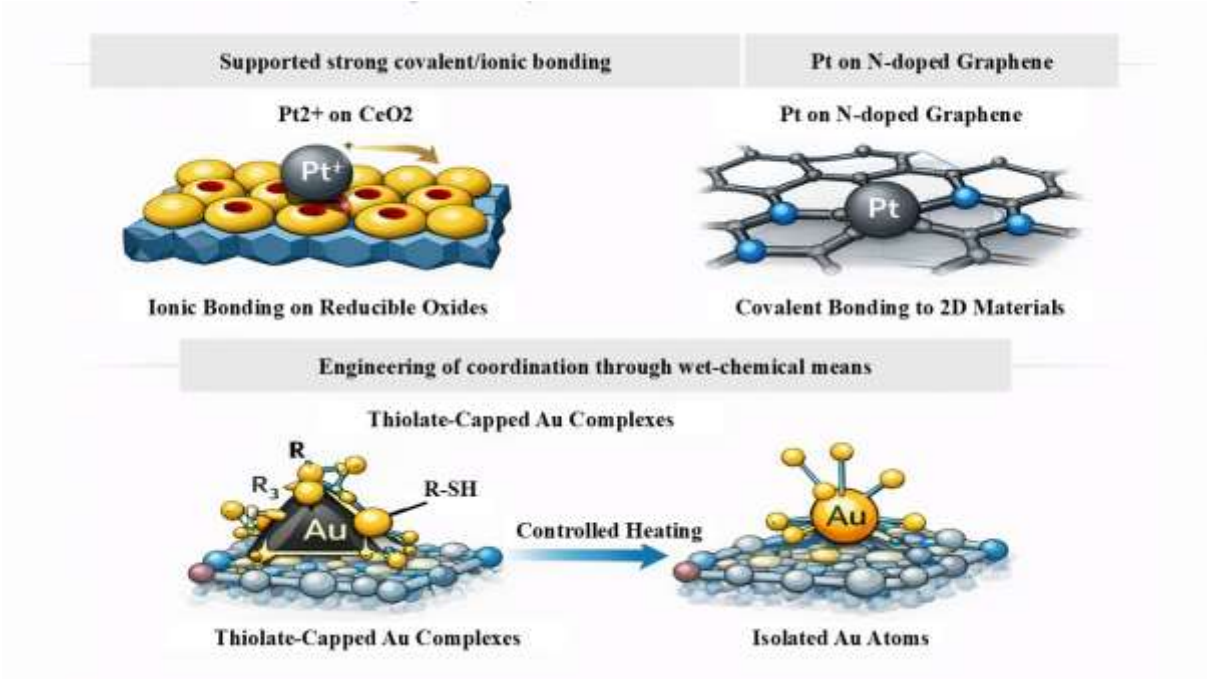


Fig.2 Stabilization of platinum single atoms through ionic bonding on reducible oxides and covalent anchoring on two-dimensional materials. Wet-chemical coordination, such as thiolate-capped Au complexes, allows for the controlled creation of isolated metal atoms when heated.

2.1.3 Mechanistic Reflections and Catalytic Applications.

SACs have been found to perform remarkably in a wide variety of catalytic reactions. In CO oxidation and preferential oxidation (PROX), SACs such as Pt1/FeO and Au1/CeO2 demonstrate high activity at low temperature, and the oxidation of CO on them occurs by a Langmuir Hinshelwood reaction involving the co-adsorption of both CO and O2 on neighbouring sites [13,21]. Similarly, in the water-gas shift (WGS) reaction, Ir1/FeO and Au1/CeO2 SACs are active in normal or even higher than the conventional catalysts with the single atoms catalyzing the dissociation of water by cooperatively catalysis between metals atom and support [22]. In selective hydrogenation, Pd1/graphene and Pt1/MoS2 SACs are highly selective in semi-hydrogenating acetylene to ethylene, which is attributed to the absence of there are no adjacent metal ensembles in them to enable over-hydrogenation [23]. Furthermore, in electrocatalytic reactions and Photocatalytic reaction, Fe-N-C and Co-N-C SACs have become promising non-precious-metal catalysts to the oxygen reduction reaction (ORR) in fuel cells, with some of the formulations matching the performance of

Pt/C ccatalysts [24]. While Pt atom on g-C3N4 or TiO2 are highly efficient co-catalysts that facilitate the separation of charge and give active sites to reduce protons [25].

2.1.4 Challenges and Limitations

Even with this impressive development, there are a number of challenges. It is challenging to obtain high metallic loadings (> 5 wt%) while maintaining atomic dispersion, which may limit volumetric activity. In addition, SACs exhibit dynamic behavior under reaction condition, where single atoms can move, form aggregates, or change oxidation state, and it is more challenging to attribute activity to a certain site structure [26]. Furthermore, there are numerous SAC synthesis methods that have limited scalability to industrial applications. Finally, reactions involving ensemble sites (e.g. C-C coupling, dissociative adsorption of N2) isolated single atoms can potentially be less active than nanoparticulate catalysts.

2.2 Design of Alloy and an Intermetallic Catalyst

2.2.1 Alloy Electronic and Geometric Effects

Bimetallic and multimetallic catalysts offer further degrees of freedom in the tuning of catalytic properties by the interactions of electronic (ligand) and geometric (ensemble) effects [27]. The electronic effect is the change in d-band center of one of the host metals when combined with a second metal to alter the adsorption strength of the reactants, intermediates, and products as per the d-band model by Hammer and Norskov [28]. The geometric effect refers to variation in the distribution and accessibility of surface atoms at certain locations (e.g., terrace, step, kink) which affects the spatial demands of molecular adsorption and reaction. In contrast to random solid-solution alloys, ordered intermetallic compounds have known crystal structures, i.e., known atomic structures, which give uniform and predictable active site geometries. PtSn, Pt3Ti, PdZn and PdGa intermetallics have demonstrated high performance in propane dehydrogenation reactions and methanol steam reforming reactions coupled with selective hydrogenation reactions [29,30]. To give one example, the site-isolation effect can be observed in PdGa intermetallic compounds: every Pd atom has no more Pd neighbors whatsoever, and no Pd ensembles are connected adjacent to each other. This geometrical isolation prevents the unselective C-C bond hydrogenolysis and retains a high level of activity in the semi-hydrogenation of acetylene [31]. Site isolation in intermetallics is a concept used to provide a deterministic method to selectivity engineering which is complementary to the stochastic site isolation of SACs.

High-Entropy Alloys (HEAs) are used as catalysts. High-entropy alloys are of major interest as catalytic materials containing five or more major elements in near-equimolar ratios. The huge compositional space and distinct thermodynamic stabilization (large configurational entropy) of HEAs present prospects of finding catalysts with heretofore unexplored levels of activity and stability [32]. The synergistic electronic effects between the elements that make up the PtPdRhRuCe have been the object of study of the research demonstrating enhanced oxygen reduction activity and lifetime of the nanoparticles over the conventional Pt/C catalysts [33].

2.3 Defect Engineering

2.3.1 Types and Roles of Defects

Crystallographic defects-such as vacancies, interstitials, dislocations, and grain boundaries-as well as surface steps, have a significant impact on catalytic properties by in creating coordinatively unsaturated sites, in altering local electronic structure, and in changing charge carrier dynamics [34]. In heterogeneous catalysis, defects have become an influential tool to be introduced and controlled. Oxygen vacancies in metal oxides (e.g., in CeO2, TiO2, ZnO, and other reducible oxides) can act as active sites of the activation of O2, allow the transfer of charge to adsorbed species, and alter the acid-base characteristics of the surface [35]. These vacancies, which is formable by means of doping or controlled reduction, is a catalytic activity descriptor of oxidation reactions. Sulfur vacancies in MoS2 and Carbon defects: The catalytic properties of MoS2 on the hydrogen evolution reaction (HER) are localised at both edge sites and sulfur vacancy sites on the basal plane. Significant enhancement of basal plane activity can be achieved by controlled desulfurization by plasma treatment, chemical etching or thermal annealing [36]. Carbon material such as graphene and carbon nanotubes contain topological defects (e.g., pentagons, heptagons, and edge sites) that provide localized electronic states, and act as catalytic sites for oxygen reduction, CO2 reduction, and other electrochemical reactions in the absence of metal centers [37].

2.3.2 Controlled Introduction of Defects.

Effective defect engineering methodology demands artificial methods that balance defect density against structural integrity. Control of vacancy concentration in metal oxides can be done by thermal treatment under controlled atmospheres (reductive, oxidative or inert). The localized defects created with spatial control are possible by ion irradiation and plasma treatment. Chemical doping brings about compensating defects (e.g. trivalent cation doping of CeO2 creates extra oxygen vacancies). Lattice mismatch strain engineering in heterostructures or core-shell structures causes defects at interfaces [38]. Effects of confinement in catalysis are described using a simple model that considers reaction orders in the framework of the elementary mechanism of reaction rates within a heterogeneous catalyst. The confinement of catalytically active sites spatially within well-defined cavities, channels or between layers presents particular effects that can radically change reaction selectivity and rates.

2.4 Zeolite Confinement

The most commercially developed type of confinement catalyst is zeolites. This molecular discrimination based on size and shape by the zeolites results in the shape selectivity, which includes reactant selectivity, product selectivity and transition-state selectivity [39].

Recent advances include: Hierarchical zeolites have interconnected micro- and mesopores, which reduce diffusion barriers but do not modify shape selectivity [40]. Single-site zeolite catalysts incorporate isolated metal ions (Sn, Ti, Zr) into the framework enabling catalysis of reaction involving Lewis acid sites (like Baeyer-Villiger oxidation, glucose isomerization, etc.) [41]. Metal clusters that have been encapsulated in zeolites and combine the reactivity of metal nanoparticles and shape selectivity of zeolite hosts [42].

2.4.1 MOF-Based Confinement

Metal-organic frameworks offer an extremely adaptable platform of confinement catalysis that includes crystallographically determined pores with adjustable dimensions (usually 0.3-5 nm), large surface areas (usually exceeding 3000 $m^2 g^{-1}$), and a chemically simple pore environment [43].

Key strategies include MOF-encapsulated nanoparticles (NP@MOF), where metal nanoparticles that are produced in MOF pores show size- and shape-selective catalysis based on the size of MOF apertures. An example of this is Pd@UiO-66, which exhibits a demonstration of molecular sieving during hydrogenation, which selectively transforms smaller substrates and excludes larger substrates [44]. Another important approach involves open metal sites in MOFs, such as HKUST-1 (Cu) and MOF-74 (Mg, Mn, Fe, Co, Ni, Zn) which contain coordinatively unsaturated metal nodes that are the catalytic sites of Lewis or redox-active [45]. Additionally, Post-synthetic modification allows the introduction of catalytic moieties (organocatalysts, metalloporphyrins, N-heterocyclic carbenes) in a site-isolated fashion into the MOF linkers. [46]. The confinement in two dimensions is another important strategy. Interlayer spaces of graphene, hexagonal boron nitride (h-BN), MXenes, and layered double hydroxides offer a much different confinement environment. Processes that take place in the 2D confined space between a metal and an overlaying 2D material have modified thermodynamics and kinetics because of the redistribution of charges, van der Waals, and limited orientations of the molecules [47]. Graphene-confined sub-nanoparticle Pt clusters exhibit high CO oxidation activity of Pt clusters as a result of charge transfer induced by the graphene overlayer that weakens CO binding and prevents CO poisoning [48].

Table 1: Comparison of Catalyst Design Strategies

Catalyst Type	Key Feature	Advantages	Limitations	Applications
Single-Atom Catalysts	Isolated atoms	High efficiency, selectivity	Low loading	CO oxidation
Intermetallic	Ordered structure	Tunable properties	Complex synthesis	Hydrogenation
High-Entropy Alloys	Multi-element	High stability	Costly	Electrocatalysis
Defect Catalysts	Vacancies	High activity	Hard control	HER, CO2RR
MOFs/Zeolites	Confinement	Shape selectivity	Diffusion limits	Biomass

3. Structure-Activity Relationships

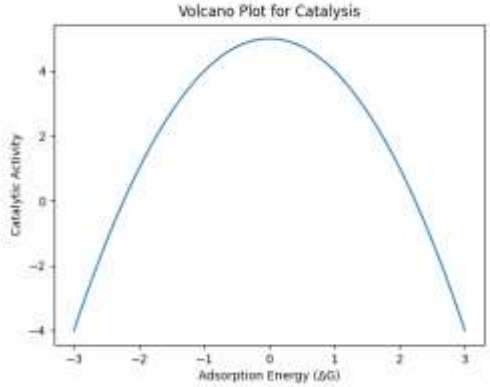
Structure-activity relationships (SAR) aim to develop quantitative correlations between the structural properties of a catalyst and catalytic activity [49]. In heterogeneous catalysis, there are several length scales in the structure, including the electronic level (d-band center, oxidation state, spin state, and charge density distribution); the atomic structure level (coordination number, bond lengths, surface facet, and density of

steps/kinks); the structural level (core–shell structure, gradient structure, composition gradient, particle morphology, size, and shape); the mesoscale structure level (porosity, surface area, support structure, and spatial distribution of the active phase); and the macroscale configuration level (pellet structure, reactor bed configuration, and washcoat thickness). One of the key tenets of SAR research is the determination of factors that are inherent to descriptors and are fundamental properties that correlate with and hopefully predict catalytic activity and selectivity [50].

3.2 Relations Between the d-Band Model and scaling.

The d-band model was invented by Hammer and Nørskov and it is a physically based electronic structure marker of catalytic activity on any metal surface [28]. Based on this model, the interaction between a molecular adsorbate and a metal surface is determined by the interaction between the valence states of the adsorbed molecule, and the metal d-band. The metallic attachment map of the d-band center (εd) to the Fermi level defines the encapsulation of anti-bonding states. The closer the d-band center is to the Fermi level, the stronger the adsorption is because there are fewer antibonding states.

It is highly successful model in which trends are explained throughout the periodic table and the impact of alloying, strain, and ligand interactions on catalytic activity can be rationalised through this framework. With Brønsted-Evans-Polanyi (BEP) relations (which provide linear correlations between activation energies and reaction energies of a family of elementary steps) combined with d-band model allow the formation of volcano plots to predict optimum catalyst combinations in a given reaction [51]. Nonetheless, linear scaling relations also have fundamental constraints. As the adsorption energy of various intermediates (i.e., OH, O, OOH in oxygen electrocatalysis) are linearly related on traditional metal surfaces, the binding strength of all the intermediates at once cannot be optimised. This scaling relation restriction limits a thermodynamic maximum of catalytic activity marking the peak of the volcano plot [52]. Violation of scaling relations, either by confinement effects, by bifunctional processes, by surface promoters or by non-metallic promoters, is thus a primary goal in the design of modern catalysts.



3.3 Size, Shape, and Facet Effects

3.3.1 Size-Dependent Catalysis

The size dependence of the catalytic properties of metal nanoparticles is extremely strong, especially in the sub-10 nm range with the edge, corner and individual facet fractions of surface atoms varying significantly with particle diameter [53]. This evolution of the structure leads to size-dependent patterns of activity and selectivity. Structure-sensitive reactions (e.g. ammonia synthesis, Fischer-Tropsch synthesis, ethylene epoxidation) are highly size-dependent that involve specific multi-atom ensembles (e.g. B5 sites to dissociate N2 on Ru) that are only readily found at certain particle sizes [54]. Structure-insensitive reactions (e.g., cyclohexene hydrogenation) exhibit not only comparatively constant turnover frequencies (TOFs) but also a size variation since the rate-limiting step can happen on any surface site. At the ultra-small scale (<2 nm), quantum size effects appear: discrete electronic energy levels, and the opening of a bandgap, and a change in the dynamics of charge carrier interactions radically change the interaction with reactant molecules [55].

3.3.2 Shape-Controlled Nanocrystals

The developments in the area of colloidal synthesis have made it possible to prepare nanocrystals of well-defined shape (cubes, octahedra, tetrahedra, nanowires, nanoplate, etc.), that can expose predominantly specific crystallographic facets [56]. This capability has been revolutionary to SAR studies: The selectivities of Pt nanocubes ({100}) facet towards cyclohexene hydrogenation/dehydrogenation, benzene hydrogenation, and pyrrole hydrogenation are dramatically different between Pt octahedra ({111}) facets [57]. The selectivities of Cu2O cubes ({100}) and octahedra ({111}) with regard to CO2 electroreduction products differ, with the facet energy of oxygen vacancy formation on the surface of each facet varying [58]. CeO2 nanorods ({110}/{100}), nanocubes ({110}), and nanopolyhedra (111}) exhibit the different activities of the CO oxidation process [59].

3.4 Operando and in Situ Characterization.

3.4.1 The Need for Working-Condition Studies.

The study of modern catalysis revealed that the geometry of a catalyst in the real reaction conditions may be quite different from the geometry of a catalyst when the catalyst is not in the reactive environment (ex situ). Such transformations as surface reconstruction, reshaping caused by adsorbates, oxidation-state changes, phase changes, and dynamic transitions between active and inactive states all occur during the reaction as temperature, pressure, and reactive gases drive these changes [7]. As such, simultaneous measurement of both the structure and spectroscopy properties of the catalyst i.e. operando characterization is paramount to the formation of credible structure activity relationships (SAR). Operando methods involves the combination of structural or spectroscopic measurements with performance monitoring and allows observation how a catalyst actually performs under the relevant conditions.

3.4.2 Key Operando Techniques

a) X-ray absorption spectroscopy (XAS), Infrared (IR), and Raman spectroscopy - XAS provides element-specific information on oxidation state (through XANES) and local coordination (through EXAFS) information under reaction conditions. It is extensively employed as a monitor of the evolution of the metal species of supported catalyst during activation, steady state, and deactivation [60]. While infrared (IR) and Raman spectroscopy are used to determine adsorbed molecules on the surface, intermediates, and spectators during a reaction. Diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS) has particularly been utilised to investigate CO adsorption configurations, formate and carbonate intermediates during CO2 hydrogenation, and the migration of hydroxyl groups on oxide surfaces [61].

b) Ambient-pressure X-ray photoelectron spectroscopy (AP-XPS)- AP-XPS enables measurement of surface composition and electronic state of material at elevated pressures [62]. Transmission electron microscopy (TEM) environmental TEM (ETEM) and gas-cell TEM allow researchers to observe catalyst nanostructure evolution in practice and observe real-time sintering, phase change, and support restructuring [63].

c) X-ray diffraction (XRD) and pair-distribution function (PDF) analysis, along with transient kinetic techniques, monitor bulk and local structural variations, which can include phase transitions, strain in the lattice and amorphization as the reaction occurs [64], and include temporal analysis of products (TAP), steady-state isotopic transient kinetic analysis (SSITKA) and modulation-excitation spectroscopy (MES), which give time-resolved information on surface occupancies, intermediates and reaction order rates [65].

3.4.3 Multimodal and Correlative Approaches.

To assess the behaviour of a catalyst, it is better to work with more than one operando technique in a single experiment, or to correlate complementary data obtained using another method under the same conditions-than to work with a single technique [66]. An example is the combination of XAS and DRIFTS which can simultaneously measure the metal speciation and the surface chemistry and connect structural dynamics with reaction pathways [67]. Newer synchrotron platforms that combine X-ray spectroscopy, scattering, imaging, and on-line mass spectrometry or gas chromatography are at the forefront of this field.

3.4.4 Dynamic and Adaptive Catalysts.

In current studies it has been revealed that most high-performance catalysts do not remain in a single structure but alter structurally with reaction conditions. For example, the oxidation state and structure of Pt, Pd and Rh catalysts can oscillate during the oxidation of CO with activity changing accordingly [68]. Restructuring of adsorbates on the surface Pt can restructure its surfaces to form platinum carbonyl clusters with the help of operando scanning probe microscopy and XAS [69]. Furthermore, at particular gas conditions, temperatures, or when loaded with metals, single atoms may be reversibly aggregated into nanoparticles, with the most stable state determined by conditions [26].

These results show that theoretical frameworks should be used that incorporate the dynamics of catalysts and self-optimise catalyst design.

4. Computational Methods of Catalyst Design

4.1 Density Functional Theory (DFT) in catalysis

Density functional theory (DFT) represents a fundamental computational approach widely used in catalysis to probe the electronic structure and reaction mechanisms underlying catalytic systems. It allows the calculation of adsorption energies, activation barriers, and reaction pathways on the atomic scale. These principles, capabilities and limitations of DFT methods for catalytic studies are discussed in this section.

4.1.1 Principles and Capabilities

This section discusses about the basic concepts and capabilities of density functional theory (DFT). The fundamental method of computational method in heterogeneous catalysis is the density functional theory (DFT). It is able to calculate adsorption energies, activation barriers, reaction pathways and electronic properties from first principles [8]. Current DFT programmes like VASP and Quantum ESPRESSO (plane-wave basis sets) and Gaussian or ORCA (localised basis sets) are able to solve surface models with hundreds of atoms with reasonable accuracy.

Key strengths include the calculation of adsorption energies to determine the strength of reactant, intermediate, and product adsorption on surfaces; transition-state searches using NEB or dimer methods to identify saddle points as well as calculate activation barriers. Electronic structure analysis, such as projected density of states (PDOS), crystal orbital Hamilton population (COHP) and charge-density difference to understand bonding. Ab initio thermodynamics used to construct surface phase diagrams as function of temperature and of gaseous pressures. Computational hydrogen electrode (CHE) system on electrochemical reaction thermodynamics as a function of potential [70].

4.1.2 Beyond-DFT Methods: Limitations and Extensions

Standard DFT, as applied with the generalised gradient approximation (GGA), is known to have a number of shortcomings. Self-interaction leads GGA has a tendency to underestimate band gaps and delocalize localised d - and f-electrons. In DFT+U corrections, this is partially corrected with regard to transition-metal and rare-earth oxides [71]. GGA also lacks van der Waals interactions, as it is not account for dispersion forces that are relevant to large-molecule adsorption and confinement. Better results are obtained with dispersion-corrected approaches like DFT-D3 and vdW-DF [72]. Strongly-correlated systems Multireference, DMFT and hybrid functionals provide better descriptions at significantly greater cost. Solvation effects are also important, where implicit solvent model (e.g., VASPsol, COSMO) and explicit solvent model are required in electrocatalysis, but they are computationally costly [73].

4.2 Microkinetic Modeling

Microkinetic models convert DFT-based energetics to experimental catalytic rates. It consists of the establishment of a kinetic network comprising all the elementary reactions, consisting of adsorption, desorption, surface diffusion, surface reactions (Langmuir-Hinshelwood, Eley-Rideal), and phase changes [74].

The significant features of microkinetic models are the development of a complex reaction network comprising of all the elementary steps adsorption, desorption, surface reactions, and diffusion. Activation energies and pre-exponential factor are computed based on DFT calculations and rate constants are estimated on the basis of transition-state theory. These models are the solution of zero-state coupled rate equations, or in more complex models, kinetic Monte Carlo simulations, to obtain the effect of space and time. The sensitivity analysis is conducted to determine the important steps of determining the rate and the important intermediates. The contribution of each step is measured by using parameters like the degree of rate control (DRC) and the degree of thermodynamic rate control (DTRC) which allow a greater insight into the activity and selectivity of catalytic reactions. [75].

4.2.2 Applications and Insights

Transformative insights have been given by microkinetic models For ammonia formation on Ru, degree-of-rate-control analysis by Campbell show that at low temperatures N2 dissociation is the limiting step, whereas at high temperatures NH3 desorption is the limiting step that explains the optimum operation conditions [76]. For CO_2 hydrogenation to methanol over Cu/ZnO/Al2O3, microkinetic analysis showes that the formate pathway is the prevailing route in bulk conditions and that long-standing mechanistic arguments are settled [77]. In electrocatalytic OER/ORR, models incorporate potential-dependent activation barriers and adsorbate-adsorbent interactions have enhanced the predictive capability of volcano plots that are used to design electrocatalysts [78].

4.3 High-Throughput Computational Screening.

4.3.1 Descriptor-Based Screening: Rapid screening of a large number of candidate materials, one can make use of a small number of descriptors that capture the key physics of a catalytic reaction. As a case study, the O and OH binding energy descriptors have been used to identify promising catalysts of non-precious-metal catalysts in O electrocatalysis [79] with descriptors being used to forecast elements generally exhibiting high catalysis potential. In addition, Systematic calculations and cataloguing of catalytic properties in large space of materials have yielded useful resources. Catalysis–Hub, The Materials Project and the AFLOW provide database of DFT-computed adsorption energies and reaction barriers of thousands of surface adsorbate interactions [80]. The Materials Project and the AFLOW also provide Buy bulk thermodynamic and electronic properties to guide the screening of catalyst stability.

4.4 Machine Learning on Catalyst Design.

4.4.1 Property Prediction Surrogate Models.

The speeds of making predictions using machine-learning models all using DFT data can be predictive of adsorption energies, activation barriers, and even other catalytic descriptors by a factor of orders of magnitude, as compared to explicit DFT calculations. Approaches include neural network potentials (NNPs) such as SchNet, DimeNet, equivariant neural networks, and Behler Parrinello symmetry function such as potential-energy surfaces predictors based on neural networks with nearly-DFT accuracy [81]. In addition, graph neural networks (GNNs) model catalyst surfaces and adsorbates with a graph, which includes information on atoms

and their environment locally. After training on millions of DFT data points, OCP GNN models are able to predict the energies of adsorbing systems in mean absolute error of about 0.2 eV [82]. Furthermore, Gaussian-process regression (GPR) and Bayesian optimization are Particularly effective on smaller data, with uncertainty metrics that are built in to leverage active learning mechanisms [83].

4.4.2 Generative Models and Inverse Design.

In addition to forward predictions, where structure is used to predict properties, generative models enable reverse design, predicting catalyst structures with desired properties directly. It is possible to suggest new combinations of alloys and surface structures with the goal of a particular catalytic reaction, generated by generative adversarial networks (GANs) and variational autoencoders (VAEs) [84]. The reinforcement-learnings frameworks can search the synthesis-parameter space to locate the best conditions of preparation [85]. There exist boundless amounts of implicit knowledge in the literature of catalysis within experimental reports. Published papers can be converted into structure-property-performance data using NLP tools to create large datasets to use in ML training and identify trends that cannot be identified based on the results of single studies [86].

4.4.3 Difficulties and Best Practises.

ML in catalysis has many challenges even after its spectacular demonstrations. There is a problem of data quality and consistency because DFT data computed with a variety of different functionals, pseudopotentials and convergence criteria are not necessarily directly comparable. The other issue is domain shift, as models that are trained on particular systems might not generalize to new chemically different materials. There is a lack of interpretability due to the fact that most ML models are black boxes; interpretable models like SHAP, LASSO, and symbolic regression are gaining popularity. [87]. Experimental validation remains critical, as ML predictions must be confirmed in the lab, and discrepancies between computational predictions and experimental realizations are still significant.

4.5 Multiscale Modeling

Catalytic processes are of length and time scales ranging between angstroms to break bonds and form bonds, to meters to design a reactor, and to hours to inactivate catalysts. To model phenomena at such scales, it is required to employ multiscale approaches to modeling based on quantum mechanical, atomistic, mesoscale, and continuum descriptions [88]:

QM/MM methods are quantum mechanical methods in which the active site is treated quantum mechanically, but the rest of the environment is treated by molecular mechanics. Computational fluid dynamics can be used to solve surface chemistry and reactor transport on top of DFT-parameterized kinetic Monte Carlo simulations. Crude-grained molecular dynamics is used to examine the interaction between catalysts and solvents, confined diffusion in microporous materials and nanoparticles stability.

5 Green and Sustainable Catalytic Processes

5.1 Energy Conversion Electrocatalysis

The Hydrogen Evolution Reaction (HER) is a catalytic reaction found in the etherification of alkene. The hydrogen economy is hubbed by electrocatalytic water splitting consumed in producing green hydrogen. The design of the HER catalyst is based on the Sabatier principle: the ideal catalysts stabilise hydrogen, neither too strongly (reducing product desorption), nor too feebly (reduction of protons). The principle creates the archetypal volcano plot of Pt at the top [89].

5.1.2 Recent Developments in Non-Precious-Metal HER and OER catalysts

More recent changes in the non-precious-metal HER catalysts have been transition-metal phosphides (TMPs) like Ni2P, CoP, FeP, and MoP and are active in acidic environments, with activities comparable to Pt because of moderate hydrogen-binding energies and high electrical conductivity [90]. The TMDs with an exemplar of MoS2 and WS2 display improved HER activity in terms of edge activation, 1T phase conversion, and defect engineering [36]. MXenes, such as Ti3C2Tx and other 2D transition metal carbides/ nitrides, have potential HER activity, which can be engineered through surface termination [91].

The electroless reaction of electrolysis is oxygen evolution reaction (OER), which represents a four-electron, four-proton transfer kinetic bottleneck in water electrolysis. Examples of benchmark catalysts in acidic media are IrO2 and RuO2, and Ni Fe layered double hydroxides (LDHs) are state of the art in alkaline media [92]. The OER catalysts can be further improved by the lattice-oxygen participation in materials (such as SrCoO-δ and BSCF perovskites) to allow direct OO bond formation through the lattice-oxygen mechanism (LOM) and avoid the traditional adsorbate-evolution mechanism (AEM), which helps to scale better [93]. Amorphous crystalline oxyhydroxides like FeOOH, NiOOH, and mixed-metal oxyhydroxides are often better than crystalline counterparts because they have more under-coordinated sites and are less rigorously structured [94]. The use of multi-element synergies to increase OER properties has been demonstrated in high-entropy oxides, including (CrMnFeCoNi)3O4 [95].

5.1.3 CO_2 Electroreduction (CO_2RR) and Nitrogen Reduction Reaction (NRR)

The conversion via CO2 reduction (CO2RR) of CO2 into useful chemicals and fuels provides a sustainable method of CO2 use. The primary difficulty is to obtain high selectivity of the desired products like CO, HCOOH, CH3OH, C2H4OH and C2H5OH and inhibit the competing hydrogen evolution reaction (HER) [96]. Some strategies used to enhance CO2RR selectivity are: Cu-based C2+ catalysts; in which the selective production of multi-carbon products by copper is taken advantage of. Cu nanocubes with the crystal face of {100} and oxide-derived Cu (OD-Cu), and Cu-organic hybrid surfaces are high-performance structures with C2 superset C2 in the Faraday efficiency of more than 70% [58,97]. CO selectivity in single-atom and molecular catalysts (Ni-N-C and Co/Fe phthalocyanines) is close to unity because they stabilize the COOH intermediate and promote desorption of CO [98]. Sn and Bi catalysts selective production of formate takes advantage of the OCHO intermediate, with excellent selectivity of more than 90% [99]. Tandem and cascade

catalysts are catalysts that convert CO2 to C2+ in a series of steps with spatially or temporally localized catalytic functions [100].

Nitrogen reduction reaction (NRR) facilitates electrochemical fixation of N2 into NH3 at ambient temperature as a possible alternative to the energy-intensive Haber-Bosch reaction. Nevertheless, the problem of reproducibility and contamination artefacts still persist as big challenges [101]. Experimental procedures have been rigorously developed, such as $^{15}N2$ isotope labeling and ^{15}N NMR quantification, switch control experiment of Ar and $^{14}N2/^{15}N2$, use of ultrapure chemicals and gas-purification traps, and statistical analysis of the ammonia production to consider contamination by the background. Remarkable catalysts are Li-mediated systems (with efficiencies of up to 50%), defect-engineered TiO2, Fe3Mo3N and molecular catalysts inspired by nitrogenase [102].

5.2 Photocatalysis

5.2.1. Design of Semiconductor Photocatalyst

Photocatalysis employs solar energy to power uphill reactions including splitting of water or CO 2 reduction and catalyse thermodynamically favourable but kinetically slow reactions, such as the degradation of pollutants. The important design considerations of semiconductor photocatalysts include their characteristics and properties, as demonstrated in Kusmer-Herbet (2012, January 25). Band-gap engineering is used to achieve visible-light absorption (Eg < 3.0 eV) and provide sufficient driving force to induce the desired redox reaction. To keep electron–hole recombination to a minimum, it is important to separate charges quickly. This can be made easier by making heterojunctions, adding cocatalysts, changing the shape of the facets, and controlling defects. Also, the kinetics of the surface must be optimized to quickly use up the charges that are created by light at the solid–liquid or solid–gas interface. This will make sure that the photocatalytic activity is high. [103].

5.2.2 Heterojunction and Z-scheme Systems and Plasmonic Photocatalysis

These Type-II heterojunctions (e.g. CdS/TiO2) as well as direct Z-schemas (e.g. g-C3N4/WO3) spatially isolate electrons and holes in the interface between two semiconductors, reducing recombination and maintaining high redox potentials [104] . In some two-component photocatalysts, the charge-transfer theory is improved by the S-step-scheme (step-scheme) heterojunction method by Yu and others [105]. In addition when excited by visible light, plasmonic metal nanoparticles (Au, Ag, Cu, Al) produce hot electrons with energy and increases the local electromagnetic fields around the particles, which allows photocatalytic reactions on non-traditional semiconductors [106].

5.3 Biomass Valorization

Lignocellulosic biomass can be converted into biofuels and chemicals through a catalytic process. The transformation of plentiful, renewable lignocellulosic biomass into both fuels and chemicals will entail selective catalytic cleavage and functionalization of C-O, C-C, and C-H bonds in complex biopolymers [107]. Key advances in this area hydrolysis of cellulose into glucose to produce a mild condition under the catalysis of solid-acid catalysts such as sulfonated carbons, acidic zeolites, heteropolyacids [108]. Lignin

depolymerization, catalysed by Ni, Ru, or Pd on carbon or oxide support selectively cleavage β-O-4 linkages in native lignin through reductive catalytic fractionation (RCF) to produce well-defined aromatic monomers [109]. Hydrodeoxygenation (HDO) is necessary to use a bifunctional catalyst with both metal hydrogenation products and acidic C-O scission sites in order to remove oxygen in bio-oil products. MoO3, WO3, and Re-type catalysts on carbon supports have good selectivity toward direct C-O hydrogenolysis, rather than unwanted saturation of rings [110].

5.3.1 CO_2 as Carbon Feedstock

The captured CO2 is converted into fuels and chemicals through catalytic conversion and released back into the atmosphere to complete the carbon cycle. CO2 hydrogenation to methanol uses $Cu/ZnO/Al_2O_3$ as the industrial standard, while $ZnZrO_4$, In_2O_3/ZrO_2 and Cu/CeO_2 have been reported to be promising as they are much more selective and stable [111]. The reverse water–gas shift (RWGS) reaction Fe, Ni, and supported noble metal catalysts converts $CO_2 + CH_4 \rightarrow 2CO + 2H_2$, providing CO feedstock for Fischer–Tropsch synthesis [112]. Dry reforming of methane (DRM) is a method that utilises Ni-based catalysts to turn $CO_2 + CH_4 \rightarrow 2CO + 2H_2$. Powerful designs should not be prone to the accumulation of carbon and sintering. The Ni/SiO_2 and Ni-Co bimetallic catalysts display superior stability [113].

5.4 Catalyst Design using the Concepts of Green Chemistry.

The green chemistry method for catalyst design include reactions in which all of the atoms of the reagents are incorporated in the product of interest, e.g. atom-transfer radical additions rather than the standard coupling reactions, the use of micellar catalysis, on-water reactions, and neat reactions to eliminate the waste of organic solvents [114]. Substitute of precious metals (Pt, Pd, Ir, Rh, Ru) with Fe, Co, Ni, Cu, or Mn-with Fe^{2+} and Mn^{2+} catalysed C-H functionalization, Ni catalysed cross coupling, and Co catalysed hydrogenation have been advanced [115]. Development highly robust recyclable heterogeneous catalysts, which can be regenerated or recovered by a magnetic process, making them less wasteful [116]. Design lower-temperature or pressure catalysts, or utilise alternative sources of energy, such as photochemistry, electrochemistry or mechanochemistry to reduce energy intensity [117].

6. Interdisciplinary Integration

6.1 Chemistry

In order to connect chemistry and materials science, it is crucial that the analytical techniques available for use are general enough as they often need to be implemented during the fabrication process. Development of complex catalytic materials involves high-end methodologies such as in-situ synthesis and characterization with techniques such as TEM, XRD, and XAS, often coupled with automated optimization routines [118]. Layer-by-layer processing makes atomic-level manufacturing possible, which gives you precise control over thickness, conformal surface coverage, and the use of stabilizers to stop sintering and leaching [119]. Bio-inspired catalyst frameworks also copy the active sites of enzymes like nitrogenase, cytochrome P450, and the oxygen-evolving complex of photosystem II in heterogeneous catalysts to make them work better. [120].

6.2 Interrelationship of Chemistry, Chemical Engineering and Autonomous Laboratories

The catalyst performance in practice attracts reliance on the intrinsic activity as well as on the transport, the reactor design and process integration. Structured catalysts and reactors such as monolithic catalysts, microreactors and 3D printed structures are used to enhance the heat and mass transfer and maintain low pressure drop [121] and membrane reactors which combine catalytic and separation i.e., dehydrogenation with H2-selective membranes are combined to drive equilibrium-limited reactions [122]. In electrochemical reactor engineering designing MEAs, optimise GDEs, and design flow cells are used to scale electrocatalysis [123] while process intensification utilise reactive distillation, sorption-enhanced reactions and chemical looping to combine reaction and separation into a single unit [124].

Autonomous and self-driving laboratories are developed through robotics, automated characterization, and machine learning, which opens previously uncharted vistas of catalyst discoveries [125]. Formulations do not necessarily require human involvement, and by using automated synthesis platforms, dozens or hundreds of formulations can be prepared and tested per day. Bayesian optimization is an information-maximising method of selecting experiments. Independent electrochemistry facilities have helped in fastening the development of CO2 and OER catalysts [126]. These automated laboratories are available to make catalyst discovery in less time and with reduced human bias and variability.

7. Conclusions and Future Perspectives

7.1 Summary of Key Advances

The catalyst design has entered a new phase of sophistication. This has been advanced by the capability of producing active sites with atomic accuracy by using single-atom catalysts, intermetallics, and defect engineering. It is also backed by profound knowledge of mechanisms made possible through operando characterization that shows dynamics of catalysts under operative condition. Experiment design and catalyst optimization are now directed by predictive computational frameworks that are premised on density functional theory, microkinetic modeling and machine learning. The increasing focus on the concept of sustainability has facilitated the use of electro- and photocatalytic methods which offer routes towards decarbon based chemical production. Additionally, the interdisciplinary collaboration of basic science and applied engineering issues allow to both design rationally, conduct tests, and scale up catalysts in order to develop a synergistic strategy that involves theoretical knowledge, experimental approaches, and application procedures.

7.2 Remaining Challenges

Catalyst design still has a number of challenges despite the tremendous progress. It is important to bridge the complexity gap since most computational and experimental studies are done on well-defined model systems, whereas industrial catalysts are subject to complex, multicomponent, impure, and pressure gradient conditions as well as deactivation effects. The stability of catalysts and their deactivation remain to be significant concerns. The behavior of performance under conditions of interest in the industry, such as sintering, coking, poisoning, leaching, and phase transformations, is to be explored further under long-term conditions. Selectivity in complex reactions has not been easily attained, especially in reactions like the reduction of CO 2 or biomass whereby there are various competing pathways. Scaling advanced catalysts such as single-atom

catalysts, shape-controlled nanocrystals and metal-organic frameworks also has issues associated to reproducibility, cost, and throughput. Lastly, testing on catalysts needs to be standardized and reproducible, particularly in developing directions such as electrocatalytic nitrogen reduction, where the protocol and benchmarking are still absent.

7.3 Emerging Opportunities

The area of catalysis is experiencing a number of exciting opportunities. Direct air capture catalysts can be used to capture and convert CO2 in one step using dual functional materials [127]. The electrification of chemical processes has the capacity to substitute conventional thermal reactor with renewable electricity, so that it can operate greenerly like e-cracking, e-reforming, and e-Haber-Bosch reactions [128]. Photobiocatalysis and hybrid biological–synthetic systems combine the selectivity of enzymes with the robustness of synthetic catalysts and the energy input from light to achieve transformations inaccessible to either approach alone [129]. Catalysis in non-conventional media including supercritical fluids, ionic liquids, deep eutectic solvents, and liquid metals as reaction media that offer unique solvation environments and transport properties [130]. Enzyme-inspired dynamic and responsive catalysts which change their structure and activity with conditions during a reaction provide control on catalysts never seen before [131]. Lastly, general chemical knowledge can also be represented by foundation models of catalysis, such as large pre-trained AI models, and refined to a specific catalytic task, much the way the language models are applied to natural language processing. [132].

7.4 Concluding Remarks

Rational design of catalysts is on a crossroad. The convergence of atomic-level characterization, first-principles computation, data science, and precision synthesis has created an unprecedentedly powerful toolkit for understanding and engineering catalytic systems. These tools need the long-term interdisciplinary teamwork between chemists that know how reactions work, that can control how materials are synthesized, engineers that design processes, and data scientists that write algorithms to realize the full potential of these tools. The catalysts produced by these concerted efforts will be instrumental in the solution of the most urgent problems of humanity, such as production of clean energy and its storage, carbon-neutral chemical production, environmental purification, and production of sustainable food. The future of catalyst design is not only the preparation of more effective catalysts, but it is the possibility to have a sustainable technological civilization.

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