ADVANCES IN CATALYSIS

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The ability to speed up chemical processes without consuming itself is known as catalysis, and it is essential to many scientific and industrial uses. This chapter presents an in-depth analysis of catalysis, starting with an overview of its basic concepts and workings. It highlights significant discoveries and technical developments while examining the historical viewpoints and significant turning points that have defined the field. The principles of catalysis are explained, including surface chemistry, reaction kinetics, and the function of catalysts in increasing the rate of reaction and selectivity. The latest advancements in the study of materials, nanostructures, and customized surface functions that maximize catalytic performance are the main topics of discussion while examining recent advances in catalyst design. Computational method advances are investigated as essential instruments for catalyst design and discovery, utilizing quantum physics and simulations of molecules to forecast. Zeolites, metallic-organic frameworks (MOFs), and catalysts with one atom are examples of novel catalytic structures and materials that are explored for their special qualities and potential uses in a variety of sectors. The chapter explores catalysis for environmentally friendly chemistry, with a focus on ecologically friendly techniques, renewable feedstocks, and green catalytic processes. Applications of catalysts in energy conversion, such as fuel cells, photocatalysis, and hydrogen production, demonstrate how important catalysts are to the development of sustainable energy solutions. To address new areas like bio catalysis, artificial based on intelligence catalyst development, and dynamic catalytic systems, recent trends and potential futures in catalysis are examined. This comprehensive evaluation of catalysis's prospects and challenges—such as deactivation of catalysts, scalability, and economic viability—offers ideas on removing obstacles and promoting innovation in the sector.

1- Introduction to Catalysis

A chemical reaction can be accelerated by a catalyst (Cuccu et al., 2023). It accomplishes this by bonding with the molecules undergoing the reaction and letting them react to produce a product that separates from the catalyst and remains unchanged, making it ready for the subsequent reaction (Zaera, 2021). The catalytic reaction can be thought of as a periodic event in which a catalyst takes part and, at the end of the cycle, returns in its original form (Shetty et al., 2020). Let's look at the catalytic reaction that produces product P when two molecules, A and B, come together (see Fig. 1.1). The binding of molecules both A and B to a catalyst initiates the cycle. Then, within this complex, A and B react to produce a product P that is likewise linked to catalyst. Product P detaches from the catalyst in the last stage, returning the reaction cycle to its initial condition (Zaera, 2021).

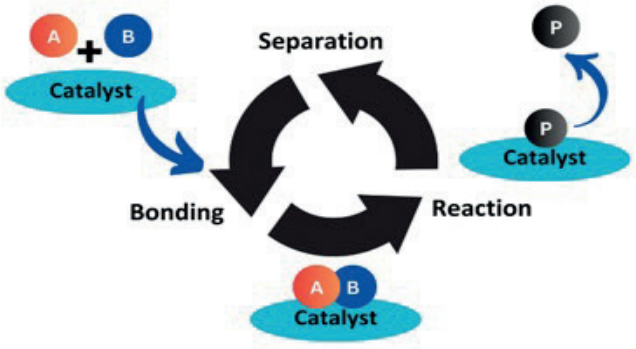


Figure 1.1. Reactant molecules attach to a catalyst, where they undergo a reaction. Afterward, the product separates from the catalyst, freeing it for use in the subsequent cycle. This is the basic process of every catalytic reaction (Zaera, 2021).

We must examine the possible energy graph in Fig. 1.2, which contrasts the catalytic and non-catalytic reactions, to understand how the catalyst quickens the reaction (Takigawa et al., 2018). The picture represents the well-known method of visualizing the Arrhenius equation for the non-catalytic reaction (Subramanian & Ragula, 2020), which happens when A and B meet with enough energy to cross the activating barrier in Fig. 1.2. Between the two reactants, A and B, and the product, P, there is a variation in Gibbs free energy of DG. The spontaneous bonding of reacting agents both A and B to a catalyst initiates the catalytic process (Takigawa et al., 2018). As a result, the complex forms in an exothermic manner, lowering free energy. The reaction between both A and B as they are attached to the catalyst then happens. Although there is an activation energy for this phase, it is far less than the activation energy for the uncatalyzed process. In the final step, an endothermic separation of product P from the catalyst occurs (Takigawa et al., 2018).

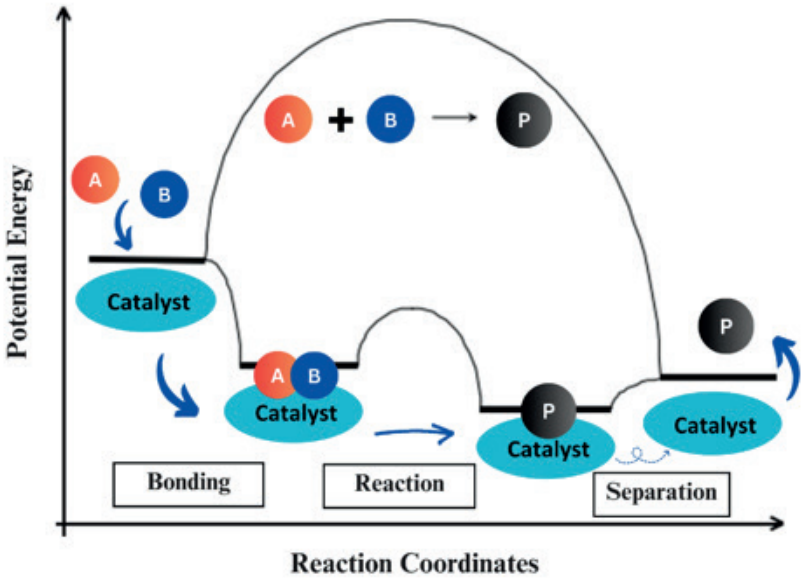


Figure 1.2. Diagram showing the potential energy generated by a heterogeneous catalytic process with a solid catalyst, gaseous reactants, and products. It should be noted that while the obstacles in the catalytic approach are significantly smaller, an uncatalyzed reaction must overcome a significant energy barrier (Takigawa et al., 2018).

Several significant points are illustrated by the energy diagram in Figure 1.2:

- The catalyst provides the reaction with a different, clearly more difficult, but energetically

far more advantageous path (Chintawar et al., 2021).

- The catalytic reaction has a much higher rate because its activation energy is substantially lower than that in the uncatalyzed process (Etim et al., 2023).
- The catalytic reaction's total change in free energy is equal to that that occurs in the uncatalyzed reaction. Therefore, an equilibrium constant of the total reaction from A + B to P is unaffected by the catalyst. A catalyst cannot therefore reverse the thermodynamic unfavourability of a process. Catalysts alter the thermodynamics but not the kinetics (Aprahamian & Goldup, 2023).
- The catalyst has the same amount of acceleration effect on the forward and reverse reactions. Put another way, a catalyst that speeds up the process of forming P from both A and B will also speed up P's breakdown into A as well as B (Noor et al., 2022).

It is currently readily apparent that there are certain situations in which using a catalyst in conjunction with reactants or products would not work:

- In contrast, if the bond between the catalyst and one of the reactants, say A, is too strong, the catalyst will be mostly occupied with species A, and B will not be available to form the product (Loenders et al., 2023). If both A and B form powerful bonds with the catalyst, the intermediate situation with A or B on the catalyst may be so stable that reaction becomes unlikely. If the bonding between reactants and catalyst is too weak, there will be very little conversion of A and B into products (Takigawa et al., 2018).
- According to Fig. 1.2, the following level is buried so deeply that the catalyst's activation energy for P formation is too high. It is believed that the reactants poisoned the catalyst (Takigawa et al., 2018).
- Similarly, it's possible that product P is too tightly bonded to the catalyst to allow for separation. Here, the catalyst gets poisoned by the product.

1.1 Solid surfaces, molecules, atoms, and enzymes can all act as catalysts

There are many different types of catalysts, ranging from molecules and atoms to big structures like enzymes or zeolites (H. Zhang et al., 2021). They can also be used in a variety of environments, such as liquids, gases, or surfaces of solids. An essential specialization that we will discuss in later chapters is the preparation of a catalyst in the ideal form and the precise examination of its composition and shape (Hughes et al., 2021). The three subdisciplines of catalysis that are typically distinguished are homogeneous, heterogeneous, and biocatalysis. We provide an example for each.

1.2 Homogeneous Catalysis

Both catalytic agent and the products of reaction are in the same phase during homogeneous catalysis, meaning that all the molecules are either in the liquid phase or, more frequently, the gas phase (Kumar et al., 2022). The study of atmospheric chemistry provides one of the most basic examples. Among other things, ozone in the environment breaks down through an interaction with atoms of chlorine (Langdon Ward, 2020).

$Cl + O_3 \rightarrow ClO_3$

$ClO_3 \rightarrow ClO + O_2$

$ClO + O \rightarrow Cl + O_2$

or overall

$O_3 + O \rightarrow 2O_2$

Although ozone can break down naturally and in response to light, a Cl atom greatly speeds up the process. The Cl atom functions as a catalyst since it exits the chemical cycle unchanged (Langdon Ward, 2020). This reaction cycle is an illustration of homogeneous catalysis since the catalyst and reactant both exist in the same phase, which is the gas phase. To create chemicals, industry employs a wide range of homogeneous catalysts in many types of processes. The carbonylation of methanol to acetic acid under catalysis by [Rh $(CO)_2I_2$]– complexes solutions are only one of numerous instances (Langdon Ward, 2020).

$CH_3OH + CO \rightarrow CH_3COOH$

Organometallic complexes are created using techniques that use molecular control in homogeneous catalysis, which is frequently used to produce delicate medications (Farina, 2023). This ensures that the reacting molecules are directed towards the desired products by the careful selection of ligands (Farina, 2023).

1.3 Heterogeneous Catalysis

Solids catalyze reactions between molecules in a gas or solution in heterogeneous catalysis. Catalytic reactions take place at the surface of solids because, unless they are porous, they are often impermeable (Rigby, 2023). Catalysts are typically nanoscale particles placed on an inactive, porous structure to make economical use of the frequently costly materials (such as $CuFe_2O_4/MgFe_2O_4$) (Fig. 1.3) (Z. Zhang et al., 2022).

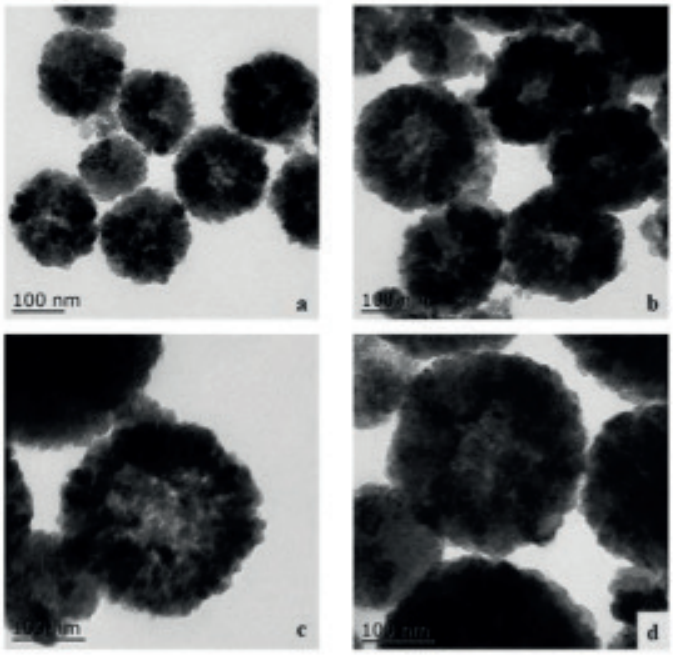


Figure 1.3. TEM images of $CuFe_2O_4/MgFe_2O_4$: (a) Cu:Mg = 1:0.5; (b) Cu:Mg = 1:1; (c) Cu:Mg = 1:2; (d) Cu:Mg = 1:3 (Z. Zhang et al., 2022).

Figure 1.3 displays the TEM images of CuFe2O4/MgFe2O4 with various Cu/Mg ratios in the precursors. It's evident that every sample created wormholes among the fine grains and hollow, spherical objects with rough surfaces. In the application process, this type of structure may help the photocatalytic reaction have a greater surface area, more active sites, simpler mass dispersion and transport, lighter penetration, and a higher quantum efficiency (Z. Zhang et al., 2022). The microspheres had a diameter of 200–300 nm, and their magnetic properties are what caused the hollow spherical formations to aggregate (Z. Zhang et al., 2022). Catalysis is nanotechnology, and catalysts are nanomaterials (Bilal et al., 2023). In the field of catalysis, nanoparticles have been used commercially for nearly a century, if we consider nanotechnology as a field of materials science

that aims to regulate material characteristics on the nanoscale scale (Lopez-Cantu et al., 2022). For heterogeneous catalysts, a variety of synthetic methods can be used to create tiny particles and maintain their stability under the frequently challenging circumstances of an industrial reactor (Abbas et al., 2024). Nanotechnology is at the forefront of modern catalysis (Noreen et al., 2022).

One of the primary processes in exhaust cleaning for cars is the catalytic breakdown of carbon monoxide (CO) on the outer layer of noble metals like rhodium, palladium, and platinum (Feng et al., 2023). This serves as an introductory example. We shall suppose that the top layer of metal has active sites, indicated by the letter "*," to explain the process. Later, we give them a proper definition (Bahtilla & Hui, 2020). The adsorption of CO and O2 on the platinum surface initiates the catalytic reaction cycle, causing the O_2 molecule to split into two O atoms (X* denotes that the molecule or atom is adsorbed on the surface, i.e. attached to the site *) (Feng et al., 2023):

$O2 + 2* \rightleftharpoons 2O*$

$CO + * \rightleftharpoons CO*$

Following their surface reaction, the adsorption O atom and CO molecule combine to create CO2, which interacts on the platinum surface extremely weakly and desorbs nearly instantly since it is very stable and very unreactive (Matsui et al., 2006):

$CO* + O* \rightleftharpoons CO_2 + 2*$

It should be noted that the catalyst's adsorption sites are freed in the latter stage, making them accessible for more reaction cycles. The chemical cycle and a potential energy diagram are displayed in Figure 1.4.

Where is the catalyst's critical influence in this cycle? Assume that the reaction occurs in a gas state without the use of a catalyst. If the temperature is raised to the point where the O2 molecule splits into 2 O atoms (radicals), the process will continue (Bakhtchadjian, 2023). When these radicals are present, the CO to CO2 conversion happens right away. About 500 kJ mol–1, or the energy needed for splitting the powerful O–O bond in O2, will be the energy needed for activation of the gas stage of the process (Bakhtchadjian, 2023). On the catalyst's surface, nevertheless, the molecule of oxygen dissociates readily during the catalytic reaction—in fact, it does so without the need for an activation energy (Etim et al., 2023). The reaction that occurs among deposited CO and O molecules, which has an energy of 50–100 kJ mol–1, is linked to the activation energy (Bakhtchadjian, 2023).

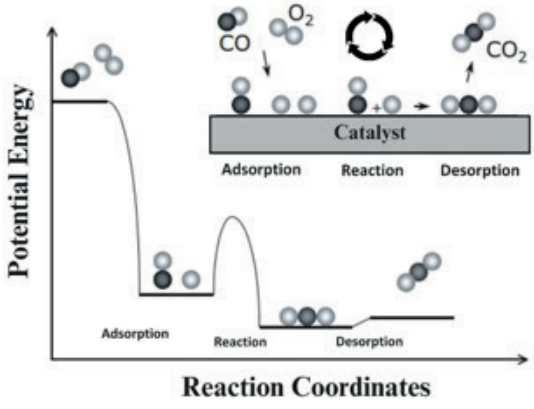


Figure 1.4. Diagram illustrating the potential energy and reaction cycle for the catalytic breakdown of CO by O_2 (Allen, 2015).

1.4 Biocatalysis

The catalysts of nature are enzymes. For the time being, it is adequate to think of an enzyme as a big protein whose structure produces an active site that is highly shape-specific (Fig. 1.5) (Palomo, 2021). Enzymes are very selective and effective catalysts because of their ideal structures, which direct reactant molecules (also known as substrates) into the best configuration for the process (González-Granda et al., 2023). Catalase, for instance, is an enzyme that catalase the breakdown of H2O2 into oxygen and water at a startlingly fast pace of up to 107 molecules of hydrogen peroxide each second (Singh et al., 2023).

$2H_2O_2 \rightarrow H_2O + O_2$ (catalase)

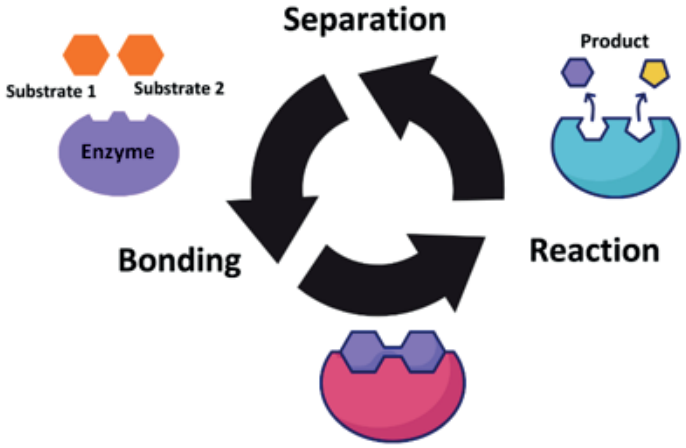


Figure 1.5. Diagram showing the reaction that is catalyzed by an enzyme. The form of the substrates that enzymes bind to or the change in phase of the reaction that they catalyze are frequently complementary. Since they are very effective catalysts, enzymes can be used as an excellent source of motivation for creating technical catalysts (Palomo, 2021).

Enzymes facilitate biological reactions at the speeds required to sustain life, such as the synthesis of proteins and DNA, the disintegration of molecules, and the energy storage in sugars (Wozniak & Brzezinski, 2023). One example that can be very interesting to students is how the body uses the enzyme alcohol dehydrogenase to convert alcohol to acetaldehyde (Zhai et al., 2023). Aldehyde hydrogenase then transforms the acetaldehyde into acetate. Some people do not have the correct type of an enzyme that breaking down acetaldehyde, which causes them to flush after even a tiny amount of alcohol (J. C. Liu et al., 2023).

2- Historical Perspectives and Milestones

Berzelius first used the term "catalysis" in 1836 (Filippi & Pizzolitto, 2022). In addition to "Affinity," he concluded that "Catalytic Force" is another force at work (J. Li et al., 2020). Catalytic contact caused the reaction to happen. Originating in Greek, the word "catalysis" means "down" and "loosen" (J. Li et al., 2020)." Catalysis in industry is not a new technique. Wine and beer have long been produced with the aid of catalysts (Uzuner, 2022). A couple of inorganic oxidation processes, such as the Deacon process (which converts HCl into Cl_2) and the synthesis of sulfuric acid, are among the earliest commercial catalytic processes (Jia et al., 2023). These procedures were created prior to the establishment of a scientific foundation for chemical reactivity. A structure for catalyst development wasn't available until Van't Hoff developed the concept of chemical equilibria (Mihara et al., 2024). This had a significant influence on the creation of a method for ammonia synthesis at the start of the 20th century, enabling a methodical, empirically supported hunt for an effective

catalyst (Emmanuel, 2024). It also marked the beginning of chemical engineering advancement that life could not exist without catalysis. All living things in the natural world, including humans, rely on enzymes, or biocatalysts, to guide the chemical reactions necessary for their survival and reproduction (X. Zhang et al., 2023). Clearly, the use of catalysis by humans to produce a product date back for further than the birth of life. However, that was a long time ago, and catalysis was not even a concept at the time ("Introduction to Heterogeneous Catalysis," 2022). For about 8000 years, yeast's enzymes have been utilized to transform sugars into goods like bread, beer, and wine (Uzuner, 2022).

Thus, catalysis—more especially, biocatalysis—has made it possible for humans to establish civilizations and lead civilized lives (Rozendal et al., 2006). Safe water and food supplies, as well as their storage, were crucial after humans began to dwell in close quarters in big numbers (Mishra, 2023). Relatively safe drinking supplies were guaranteed using yeast to generate alcoholic beverages while also inhibiting all other pathogenic microbes. Similarly, yeast-based bread produced products that could be stored (Cabello-Olmo et al., 2023). Another frequent use of catalysis is the growth of Lactobacillus and related organisms that overpower pathogens while producing acidic media and thereby suppressing all other microbes (Balakumaran et al., 2021). The process of catalytic creation of lactic acid is utilized in the production of yoghurt, cheese, and numerous other dairy-based goods to preserve milk, as well as in the production of salami and numerous other kinds of food (Dahiya & Nigam, 2023). By wrapping the meat in papaya leaves, the meat was softened and rendered more palatable for human ingestion thanks to the proteases found in the leaves (Obajuluwa et al., 2020).

Catalysis as a concept began to take shape in the second half of the nineteenth century (Loenders et al., 2023). Depending on whatever solid was added, it was found that ethanol might either break down into ethylene or acetaldehyde, which has a strong odor (Fustier et al., 2011). We now understand that while oxides with acid activity cause dehydration, metals catalyze dehydrogenation (Cabello-Olmo et al., 2023). The sensor that can identify explosive gases was the first application that was created by humans, but at the time they were unaware of the notion. With the help of a teenage Michael Faraday, Davy discovered in 1817 that H_2, CO, and CH_4 in the air could be detected by a heated Pt wire because the oxidation of the gases would cause the wire to light up with heat (Balakumaran et al., 2021). This made it possible to identify dangerous gases in mines for coal before their concentrations rose to the point where an explosion was possible. Based on this, the Miner's lamp—a crucial safety tool in mines for coal at the time—was created. Inspired by the Greek word for "loosen," JJ Berzelius originally coined the term catalysis in 1835 and explained the underlying mechanism (Dahiya & Nigam, 2023). It was suggested that the catalyst could cause organic materials, such as the elements in mine gas, to decompose (Obajuluwa et al., 2020). The idea was not fundamentally dissimilar from the idea of dissociation adsorption in surfaces today.

3- Fundamentals of Catalytic Processes

Relevant economic limitations exist for catalyst expenses, catalytic efficiency, and process selection (Fustier et al., 2011). Enhancing the catalyst does not always result in a system that is useful in real-world scenarios. It's interesting to note that new possibilities for catalyst choice are directly correlated with our grasp of molecular prediction, as the catalyst choice issue will demonstrate (Elphick, 2021). Mass and heat exchange play a major role in extrinsic kinetics, which also influences reactor selection and catalytic performance. The relationship between the energy content of the final product and the raw material plays a major role in the energy conversion technology process selection (Ren et al., 2020).

3.1 Selection of Catalyst

The creation of a computer method for assessing and forecasting the catalytic activities of heterogeneous catalytic systems is a significant contribution of computational catalysis (J. Xu et al., 2021). This approach makes use of the relationship between a calculated reactivity descriptor and a

measured rate of a reaction. This approach takes advantage of the physical-chemical interpretation of the behaviour like a volcano (Mañosa et al., 2023). The Sabatier principle has led to this. The maximum in the volcano curve happens when the rate of reactant activity and the rate of product desorption are equal, if one utilizes the interaction intensity of the reactant with the catalyst as a reactive parameter (Figure 3.1) (Králik, 2014). The rate of reaction rises as you increase interaction energy to the left side of the volcano and reduces with rising reaction energy to the right. The total catalytic rate exhibits a maximum rate at the reactivity descriptor's optimal value (Mañosa et al., 2023).

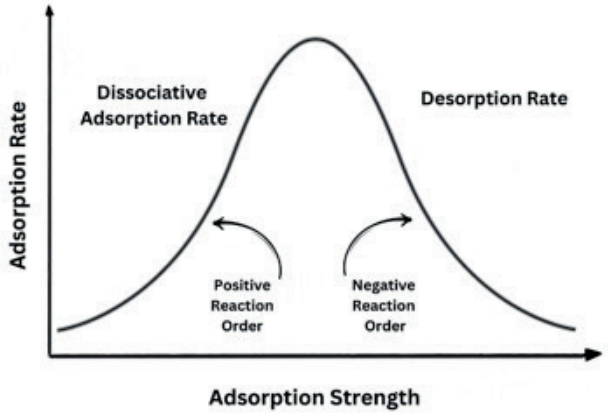


Figure 3.1 According to Sabatier's concept of catalytic reactivity, the rate of reaction peaks when the reagent and catalyst have the best possible relationship (Králik, 2014).

Using a linear activated energy–reactivity descriptor connection of the Brønsted type for elementary reactions on the surface is the second component of the extrapolative rate prediction (J. Xu et al., 2021). A thermodynamic quantity such as the chemical reaction energy of a crucial fundamental reaction step is employed as a reactivity descriptor. This is known as the Brønsted–Evans–Polanyi relation (BEP) for surface reactions (Chun et al., 2020).

In Figure 3.2a, one such relationship is depicted. Plotting the calculated energy of activation for CO dissociation, or C–O bond cleavage, versus the total of the adsorbed C and O adsorption energies is done (Andersson et al., 2006). There are corrugations on the surface. The BEP proportional constant, or the curve's slope, is almost one. It shows that the C–O bond is extremely weak in the phase transition state and that the framework of the dissociated state and transition state are extremely comparable. When there is a substantial amount of available experimental data, the appropriate descriptor can be utilized to create a volcano curve once the reliability of the BEP relation for an important reaction stage in a catalytic reactions step has been confirmed (Stratton et al., 2023). Such information can also be computationally generated through the application of micro kinetic methods for modelling of the innate catalytic rate.

Figure 3.2b displays a plot of the catalytic reaction's experimentally determined rate constants:

$CO + 3H_2 \rightarrow CH_4 + H_2O$

as opposition to a reactivity descriptor defined as the total of the breakdown products Ediss adsorption energies. The Sabatier concept is followed in finding a volcano-type response rate dependence. The reactivity descriptor's optimal value is nearest to 0 (Andersson et al., 2006).

The ability to access a volcanic curve like the one shown in Figure 3.2b makes it possible to computationally test many metal combinations. The total of C and O's adsorption energies (Ediss) for various metal compositions must then be determined. This allows for the computational analysis

of the reaction kinetics for a wide variety of metal combinations. Using this technique, substitutes for the pricy Co and Ru metals that exhibit peak methane reforming reaction performance have been identified (Andersson et al., 2006).

The application of these variables to determine the preferred material from an economic standpoint is demonstrated in Figure 3.3 (Védrine, 2017). An example of an Ediss Pareto plot of a specific metal combination vs its price is displayed. The material performs at its best when Ediss is zero (Magnuson & Ma, 2022). This will never match the best deal unless very rare circumstances arise. A trade-off between the best performance and the lowest process can be made using the Pareto plot. The alloy FeNi3 has the lowest price and near-maximum performance, according to the Pareto plot (Magnuson & Ma, 2022).

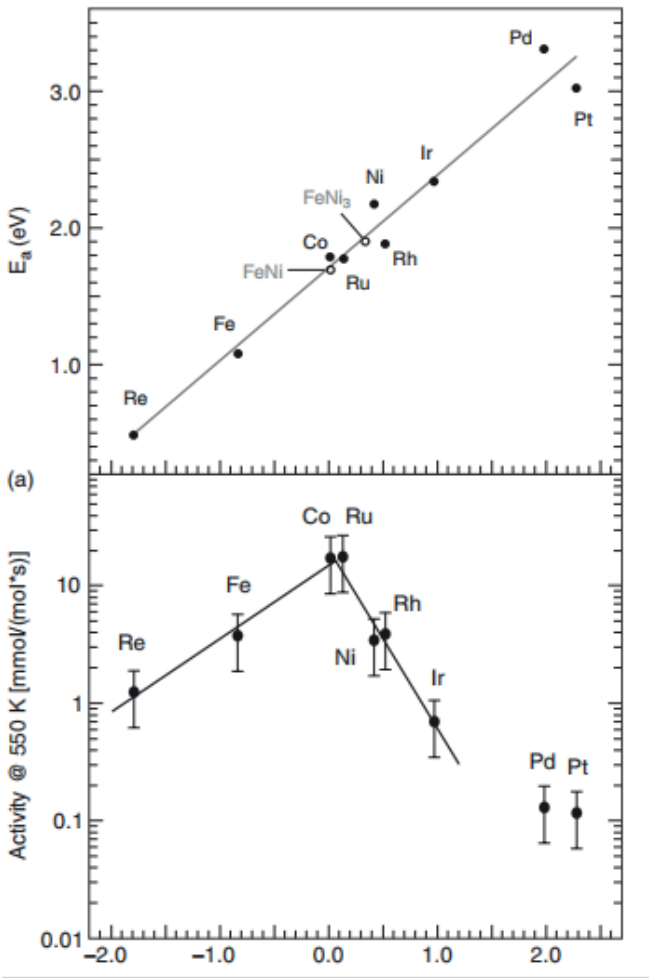


Figure 3.2 (a) BEP connection between the CO dissociation energy and the activating energy for CO dissociation, Ediss. **(b)** Catalytic activity measurements for supporting metal catalysts are displayed against Ediss. The RPBE exchange correlation was utilized in the computations on stepped fcc (211) metal slabs that were periodically repeated and had 12 layers in the (211) direction (Andersson et al., 2006).

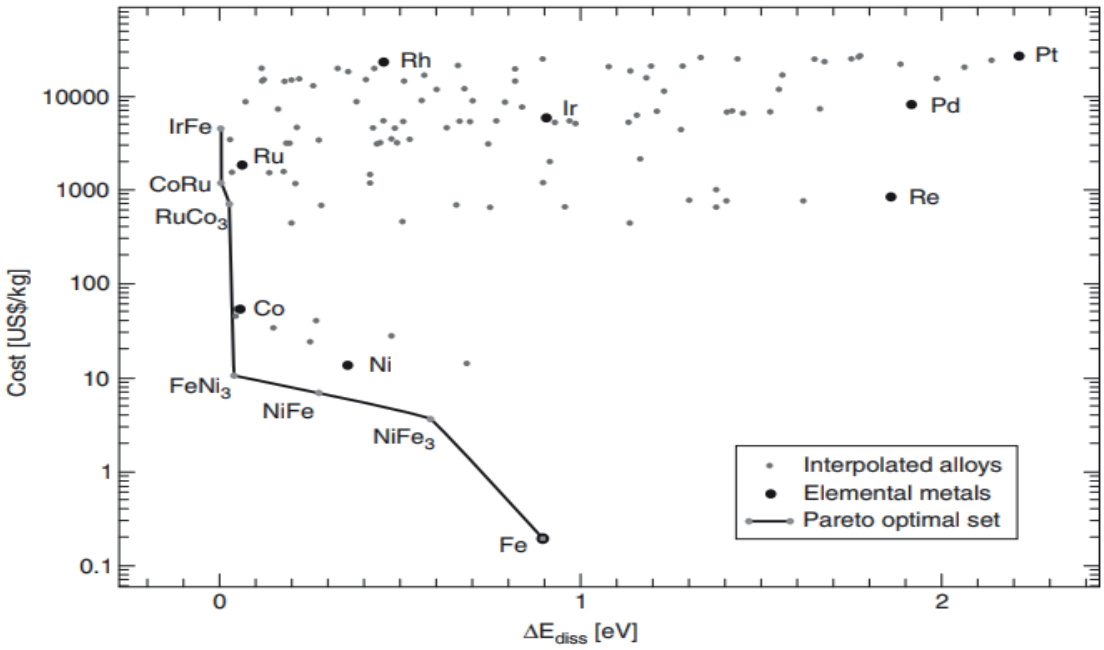


Figure 3.3 The activity measure's Pareto plot ΔEdiss = |E′diss − Eoptdiss | and the price of 117 bimetallic alloys and elemental metals (Védrine, 2017).

3.2 Choice of Reactor

It's not always the case that the catalyst with the highest activity is also the most practical. Extrinsic kinetic characteristics like mass and heat exchange rates also influence the total rate of a catalyzed reaction. Reactivity regimes for three processes are contrasted in Figure 3.4 (Ountaksinkul et al., 2022). The reservoirs for gas and oil are produced by petroleum geochemical processes. These processes have an extremely low space-time yield. Additionally, a comparison between the ideal operating window for commercial catalysis and the biochemical processes involved in fermentation is presented (Moulijn et al., 2011). Take note of the three order of magnitude disparity between biological and industrial catalysis. The trade-off between two factors accounts for the industrial process' optimal window. One is a catalyst's intrinsic rate, which should ideally be maximum (Mbatha et al., 2021). The rate at which mass may be transferred from or into the catalyst or the quantity of heat that needs to be added or removed, however, might become limiting variables when a reaction reaches extremely high rates. These restrictions are imposed by reactor design. Usually, the process is run at its best when production rate is constrained by mass and heat transmission (Mbatha et al., 2021). Then, the allowable limitation values are determined by intrinsic kinetics. It seems obvious that production increases with improved control and augmentation of the extrinsic kinetic parameters (Moulijn et al., 2011).

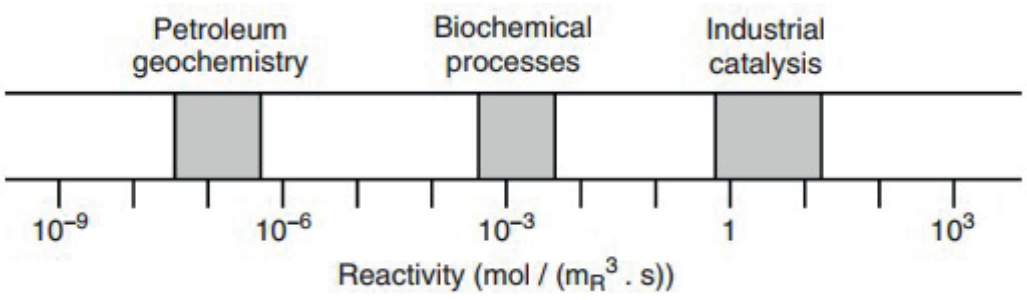


Figure 3.4 Reactivity thresholds for many chemical reactions (Moulijn et al., 2011).

3.3 Choice of Process

When choosing a process, thermodynamics and material efficiency are crucial factors. Sheldon et al., 2022, established the idea of Atom utilization to gauge material efficiency (Sheldon, 2022). The main concept is to count the total amount of atoms in the starting materials divided by the number of atoms in the product to determine how much waste material is produced. To assess effectiveness on a weight basis, it is helpful to translate the Atom utilization number into a ratio of weight for practical reasons (Sheldon, 2022).

The choice of reactor and catalyst can affect the effective Atom utilization. It is dependent upon a reaction's selectivity (Y. Zhang et al., 2022). We show this in Figure 3.5 for epoxidation reactions to ethylene (Pilli & de Assis, 2018). Using Cl2 and Ca(OH)2 as reactants, the traditional pathway passes through the intermediate chlorohydrin. 25% of atoms are used, and the waste product is CaCl2 (L. Wang et al., 2023). Ethylene epoxide is optimally produced with 100% selectivity using the Ag-based catalytic method. There is 100% atom utilization. When the reaction is conducted with 90% selectivity in practice, 77% of the atoms are effectively utilized. It serves to highlight the significance of catalytic processes. This figure remains notably greater compared to that of the chlorohydrin pathway (L. Wang et al., 2023; Y. Zhang et al., 2022).

Thermal efficiency is crucial when handling transformation operations like turning petrol or coal into liquid fuels for transportation. This is calculated by dividing the product's combustion heat by the total amount of feedstock consumed (Y. Zhang et al., 2022). For example, oil refineries usually have a 90% thermal efficiency. In comparison, the heating efficiency of producing a non-fuel product like methanol, which has an energy efficiency of only 67%, should be considered (L. Wang et al., 2023).

De Jong et al., 2022, cited two crucial guidelines for effective processes (de Jong et al., 2022):

- Reducing the amount of process stages
- Variation in the hydrogen content between the feed and the final product

The transformation of coal or natural gas into liquid carriers of energy serves as an example of the significance of hydrogen content (Tashie-Lewis & Nnabuife, 2021). The transformation of natural gas to hydrogen-rich paraffinic compounds has a significantly better heating efficiency than the transformation of coal, as shown in Figure 3.6 (Boretti & Banik, 2021; Tashie-Lewis & Nnabuife, 2021).

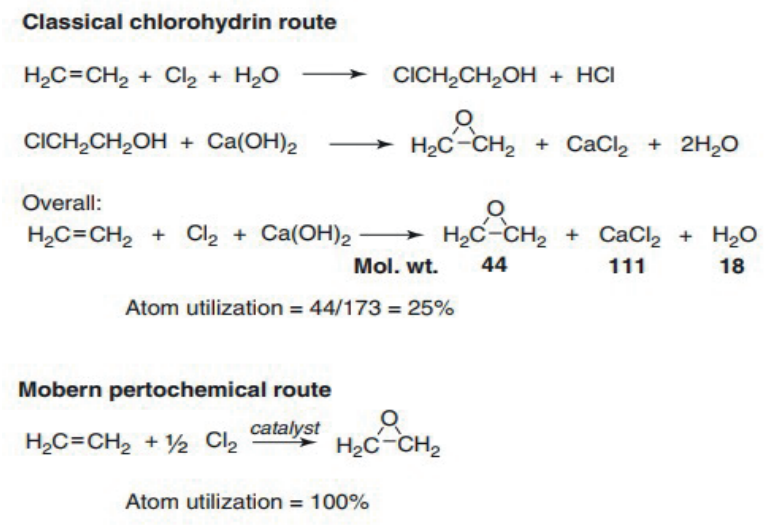


Figure 3.5 The contemporary petrochemical approach uses 100% atom utilization, while the traditional chlorohydrin route uses 25% (Pilli & de Assis, 2018).

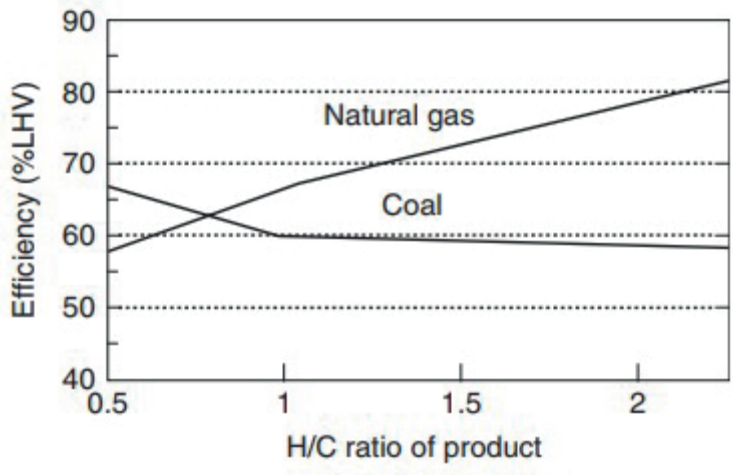


Figure 3.6 Maximum thermal efficiency of the synthesis gas into hydrocarbon in synthetic fuels (Boretti & Banik, 2021; Tashie-Lewis & Nnabuife, 2021).

4- Recent Developments in Catalyst Design

Every chemist is aware of how important it is to have an effective catalyst to maximize stereo- and regioselectivity and increase reaction rate (Cuccu et al., 2023). A variety of techniques, including the simulation of various catalyzed processes, trial and error methods, screening of preexisting catalyst libraries, and, lastly, sound chemical intuition and understanding, are used in the search for new catalysts (Zhuang et al., 2024). Most of the time, a mix of these strategies is used, and serendipity also plays a significant part. Either way, controlling chemical reactions using precisely engineered catalysts—that is, molecules or material that are both effective and may meet other crucial needs like cheap cost and minimal environmental impact—is the very ambitious goal (Bollini et al., 2023).

A search of the Scopus database was conducted to determine the significance of rationally tailored catalysts. The search yielded 43,897 entries related to the string “Catalyst AND Design” for the years 1928 to 2021; of these, 20,838 entries are from the years 2016 to 2021, indicating a sharp rise in interest in and work on catalyst design over the previous five years (Figure 4.1a) (Kobayashi & Sunada, 2020; Ma et al., 2019). When the full term "Catalyst AND Design AND Strategy" is entered into the search, 4087 results covering the years 2016–2021 are identified when strategy is included (Figure 4.1b) (Kobayashi & Sunada, 2020; Ma et al., 2019). Significantly, both graphs show that the number of works is rising annually, a sign of the scientific community's interest in the methodical and directed hunt for new catalytic systems. Computational approaches are a valid assistance in this case for various reasons. First, precise quantum chemistry methods have produced quantitative energy and kinetic understanding by revealing mechanistic insights of both simple and complex events within the past 20 years (Ta et al., 2021). These days, (super) computers can be used to study chemical reactions involving complicated systems, thanks to the remarkable advancements in silicon technology. In conclusion, the use of machine learning to screen vast collections of chemical substances is regarded as a standard best practice for investigating possible activities in silico or extracting key properties for designing functional molecules (Zhuang et al., 2024). With the help of all these data, we can predict that chemists will soon be able to design effective catalysts and create them in the laboratory with the least amount of expense and work.

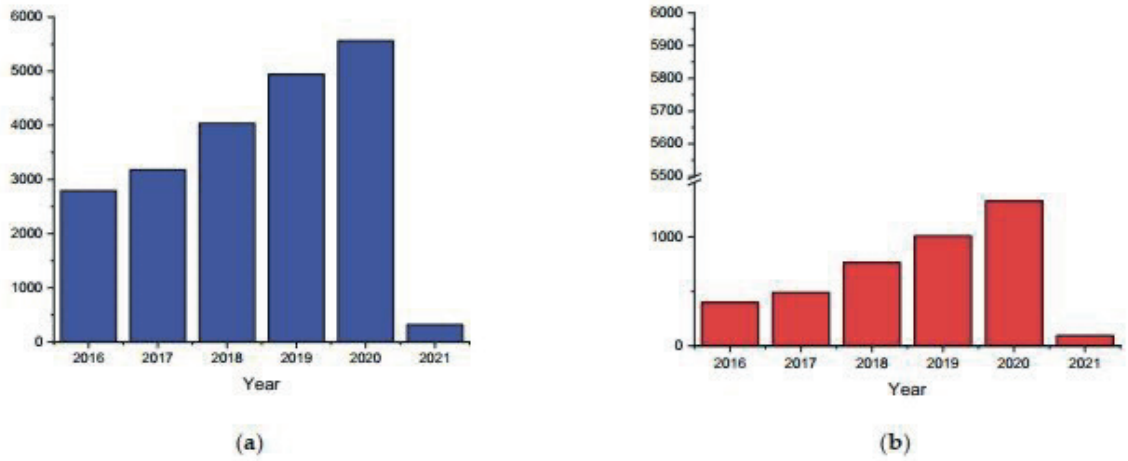


Figure 4.1 Outcomes of a Scopus database search restricted to the years 2016–2021: The search terms "catalyst AND design" in (a) and "catalyst AND design AND strategy" in (b) (Ma et al., 2019).

A method for shielding palladium catalysts from Sulphur species has been described by Betti et al. (Betti et al., 2021) and used in the catalytic oxidation process of methane. Different researchers have explored and analyzed in detail the issue of asymmetric olefin epoxidation using salenMn immobilized on graphene oxide as a catalyst ("Advanced Strategies for Catalyst Design," 2021; Orian, 2021). Inspired by the silicon analogue, Kobayashi and Sunada have reported the production of a four coordinated Fe(II) digermyl complex that is used as a catalyst in the dehydrogenation of ammonia borane (Kobayashi & Sunada, 2023). According to Hernández et al., introducing Pt to the Ag/Al_2O_3-WO_x catalyst improves the elimination of NO_x utilizing C3H8 and H2 (González Hernández et al., 2020). Muangmora et al.'s study uses Mn/Ti nanorods to remove fundamental mercury in the form of SO2, demonstrating how the TiO_2-coated Mn is protected from SO_2, an undesired deactivation (Muangmora et al., 2021). WU et al.'s review paper focuses on the difficulty of developing a nontoxic catalyst for acetylene hydrochlorination, which is catalyzed by $HgCl_2$ supported on activated carbon (WU et al., 2021). Alternative options are evaluated, and benefits and problems are critically discussed, for noble as well as non-noble metallic and nonmetal catalysts. The research on alternatives to petroleum products derived from fossil fuels was documented in the article by WU et al. The authors have demonstrated the production of 22-carbon tricarboxylic acid and its ester using the Diels-Alder reaction, commencing with polyunsaturated fats (PUFAs) and their corresponding esters, fumaric acid and fumarate. A catalyst has been employed with iodine (WU et al., 2021). Carlucci et al. have worked on developing methods to turn waste cooking oil into biofuels, and they have been successful in maximizing the conditions of the reaction (acid catalysis) to achieve high yields of up to 99% (Carlucci, 2021). In their investigation into the removal of chemical waste from wastewaters, Rottach et al. suggested the contact glow discharge electrolysis (CGDE) method, which has the potential to be a low-cost solution (Rottach et al., 2023). Lastly, two theoretical investigations have been given by Kim et al. and Orian et al. The first one involves the asymmetric cyanation of olefins using ethyl cyanoformate, which is catalyzed by Ti(IV). The second one involves the cycloaddition of acetylene [2+2+2] to benzene, which is catalyzed by Rh/Cr indenyl fragments. It is clear from the precise explanation of the reaction processes and the activating strain model that the time is right for an exacting and quantitative in silico catalyst design (Rottach et al., 2023).

5- Computational Approaches in Catalysis

In addition to offering a flexible toolkit for researching the mechanistic specifics of catalytic reactions, computational chemistry has the potential to produce useful approaches that will facilitate the logical in silico design of catalysts (Kee, 2023). The system's ubiquitous activity and complex

electronic structural affects. Traditionally, chemical intuition and professional advice of the researcher have been crucial to computational investigations on catalytic reactions (Lledós, 2021). The human-bias from computational catalysis investigations may be eliminated thanks to recent advancements in sophisticated automated reaction path analysis techniques. All initiatives for the construction of sustainable chemical technologies that are atom- and energy-efficient rely heavily on catalysis. Today, nearly all consumer goods, from fertilizers and transportation fuels to fabrics and medications, are produced using inexpensive oil, gas and coal feedstocks, which are vital to civilization (Iroegbu & Ray, 2021). Dependence on these renewable feedstocks raises the risk of political and economic instability on a worldwide scale and is linked to significant greenhouse gas emissions, raising concerns about climate change. It is obvious that this scenario leads to an unsustainable future. To make it possible to directly use alternative renewable raw materials and to improve the efficiency and environmental friendliness of currently in use technologies, new ones must be invented and developed quickly (Mariotti et al., 2020). The move to more robust and effective catalytic systems, ideally composed of elements that are abundant in the earth, is implied by attempts to make catalyst utilization more sustainable (Kumar et al., 2022). These endeavors should be performed in tandem with work towards the feasible use of chemical feedstocks.

Computational chemistry has emerged over the past 20 years as a major component of catalysis research and has made a name for itself alongside common laboratory methods like infrared spectroscopy (IR), nuclear magnetic resonance (NMR), and X-ray diffraction (XRD) in the catalysis toolbox (Rivera-Torrente et al., 2020). The advancement of our basic comprehension of catalytic events has been greatly aided by computational modelling and molecular simulations (Lledós, 2021; Ta et al., 2021). To provide an atomic structure for the analysis of spectroscopic data and the clarification of catalytic mechanisms, computations have become essential. The study of chemical reactivity, the analysis of intricate reaction pathways, and the modelling of catalytic reaction kinetics are all best served by state-of-the-art quantum chemical methodologies, especially the density functional theory (DFT) approaches (Ugwu et al., 2022). Important instructions for the creation of novel and enhanced catalytic systems are provided by theoretical research. The availability of easy quantum chemical and molecular modelling software, which makes it possible to practice quantum chemistry without the need for extensive programming skills or specialized theoretical expertise, has made computational chemistry more widely applied (Mazzola, 2024).

These days, atomistic DFT modelling results are widely used not only by theorists but also by a wide spectrum of experimental catalysis groups, who use the data in support of mechanistic proposals gained from the experiments (Morales-García et al., 2021). The enormous achievement of near-chemical precision that can be reached with the current computational methodologies has made a direct relationship between the outcomes of molecular modelling and experimental data a standard practice (Kee, 2023). In computational chemistry, accuracy is typically defined as the ability of a given approach to compute certain fundamental chemical properties in relation to experimental or extremely precise theoretical conclusions(L. Wang et al., 2023). The total accuracy of practical calculations involving catalytic systems is also highly dependent on the model's quality, or how well it captures the crucial chemical characteristics of the reaction or feature under consideration (J. Xu et al., 2021). The approach (degree of theoretical approach) and model accuracies (amount of chemical information incorporated in the model) naturally trade off with one another.

5.1 Competition in computational catalysis between model and method accuracies

Since electronic structure theory is the only one that can explain the fundamental process of catalysis, which is the breaking and creation of chemical bonds, it plays a crucial role in the understanding of intricate reaction mechanisms (Rocchigiani & Bochmann, 2021). The discussion of computational chemistry's correctness in relation to research on catalytic structures based on three-dimensional transition metals is the main objective of this section. Within this framework, the issue of computational accuracy can be perceived as consisting of two primary elements: (a) the precision of the technique utilized to ascertain the electrical composition of the chemical system, and

(b) the precision or caliber of the chemical model utilized to explain the fundamental phenomena that underlie the feature significance of the chemical system (Keith et al., 2021). Achieving the optimal levels of models and method accuracy at the same time is frequently unattainable due to the intricate chemistry and electrical structure of these catalytic systems (Rey et al., 2024). As a result, several apologies and simplifications must be made to define the model system and describe the electronic structure. The selection of a density functional, the degree of correlation applied in post-Hartree-Fock techniques, or the dimensions and kind of the basis set are a few examples of these methodological approximations (Determan & Wilson, 2024). Crucially, the selection of the concept level dictates how comprehensive the set of basic physical occurrences is that one may dependably use to explain the computing itself. This highlights the need of accurately calibrating these methods and estimating the errors incorporated into the computational study in real computational catalysis research (Jung et al., 2022). As a result, we will offer suggestions for using electrical structure theory techniques to produce (semi)quantitative results in this section. To make the system tractable and achieve the required computational accuracy, the model approximations are mostly connected to the necessity of reducing the model's size in a general way (i.e., the number of atoms, size of the configurational or reactive space probed in the simulation, etc.) (Bürkner et al., 2023).

5.2 Accuracy of Quantum Chemical Methods - Density Functional Theory (DFT)

Since density functional theory (DFT) has a wide range of applications in computational catalysis, it will be covered first. DFT has become quite popular because of its simplicity and application, even though historically it was brought to chemically relevant problems considerably later than the other key family of quantum chemical approaches, the wave function theory (WFT) methods (Butera & Butera, 2024). Since DFT has been thoroughly covered in many great textbooks and review articles, this chapter provides a very brief overview of the method's fundamentals here to lay the groundwork for our discussion of the benefits and drawbacks of related methodologies for researching realistic catalytic systems (Ugwu et al., 2022).

The two Hohenberg-Kohn theorems, which assert that the ground-state energies can be calculated variationally and can only be determined from the electron density, are the basis of density functional theory (DFT) (Determan & Wilson, 2024). According to the second theorem, an energy larger than or equivalent to the true potential can be estimated if the exact definition of the density is known. Kohn and Sham developed a method that served as the foundation for the current Kohn Sham DFT (KS-DFT), which is akin to the self-consistent field (SCF) method used to solve the Hartree-Fock (HF) equations (Belleflamme et al., 2023).

The majority of practical DFT approaches now use KS-DFT, which assumes that there are no interacting electrons in the system (Belleflamme et al., 2023). The electrons that have an electron-to-electron correlation create the genuine (full) ground-state density. Then, the Eigen function is a conventional Slater determinant created by individual one-electron operations, the eigenvalue is a sum of one-electron eigenvalues, and the Kohn−Sham operator, the DFT counterpart of the Fock operator, is written as the total of one-electron operators (Izsák et al., 2023). The density, or electron density, is an expression of three-dimensional spatial coordinates, and the function that sums the potential and kinetic energy operators is a density functional (Kocák et al., 2023).

Utilizing machine learning to expedite the chemical space exploration is an alternate strategy that has begun to get a lot of traction (Keith et al., 2021). It is anticipated that data-driven approaches would hasten the process of identifying important characteristics that can serve as catalytic descriptors and aid in computational catalyst design (H. Li et al., 2023). To create a thorough theoretical foundation for computational catalysis, those methods can be integrated with the subjects (new electronic framework theory methods, complicated modelling, computing of many reaction paths, and reaction network analysis) (Bernales et al., 2018).

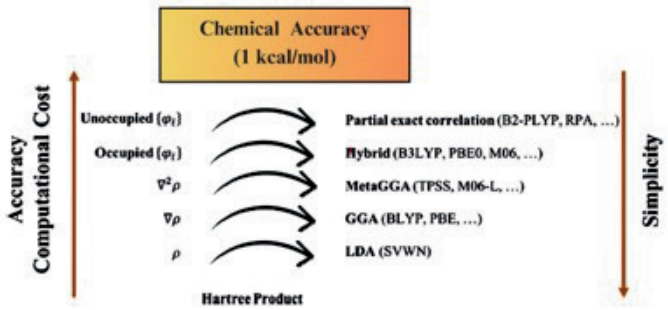


Figure 5.1 Diagrammatic representation of the different DFT approximations sorted by decreasing simplicity, increasing accuracy, and increasing processing expense. For every rung, a few popular and representative functional are provided (Olatomiwa et al., 2023).

6- Novel Catalytic Materials and Structures

In heterogeneous catalytic reactions involving the transformation of chemicals produced from biomass, the breakdown of metal catalyst is a frequent occurrence that can have a direct impact on the pace, conversion, and selectivity of the reaction (Mo et al., 2023). To avoid deactivation, improve catalytic performance, and increase selectivity towards the intended product, catalyst design is crucial (Tafete & Habtu, 2023). The design of supported metal catalysts, with an emphasis on alloy, micro-structure, or hybrid composites, which are functionalized supports with appropriate microstructure or strong interaction, and quite a few other novel structural catalytic materials, has been aided by the development of synthesis techniques and characterization technologies (Song et al., 2024). In this chapter, we primarily focus on newly developed structural catalytic substances with exact crystalline structures. These materials include metal nanoclusters and porous materials like zeolites, MOFs, and COFs.

6.1 Porous materials

(I) Zeolite

One type of naturally occurring alum inosilicate with evenly spaced pores is called zeolite. Another name for synthetic zeolite is molecular sieve (Kianfar, 2020). Ax/n (SiO_2) (AlO_2) x·mH_2O (A = cation) is the general formula for a molecular sieve. Its four-junction framework is TO_4 (T = Si, Al, etc.) (Carreon, 2008). Numerous configuration types result from the various TO_4 connection modes. 235 varieties of both natural and synthetic zeolites have been identified thus far, with each kind given a three-letter designation by the International Zeolite Association (Z. Wang et al., 2012). Figure 6.1 depicts the architecture of a few widely used zeolites (D. Yang et al., 2021). The frameworks of these rings are made up of varying diameters, which match the pore windows. Zeolites are classified into four groups based on the biggest pore size: small-pore (≤8-ring), medium-pore (10-ring), large-pore (12-ring), and extra-large pore zeolites (>12-ring) (Meier, 1986). Zeolites with diverse shapes are capable of selectively producing certain products by catalysis, thanks to the unique spatial constriction of their pores and the distinct Brønsted (B)/ Lewis (L) acid active sites in their structures (Kianfar, 2020). As a result, zeolites are frequently employed as heterogeneous catalysts, playing a significant role in both traditional petrochemical industries and cutting-edge sustainable processes including the conversion of biomass, purification of water, C1 molecule conversion, and others (Carreon, 2008). Zeolites can also be used as supports to create multifunctional composites with superior catalytic capabilities (Z. Wang et al., 2012).

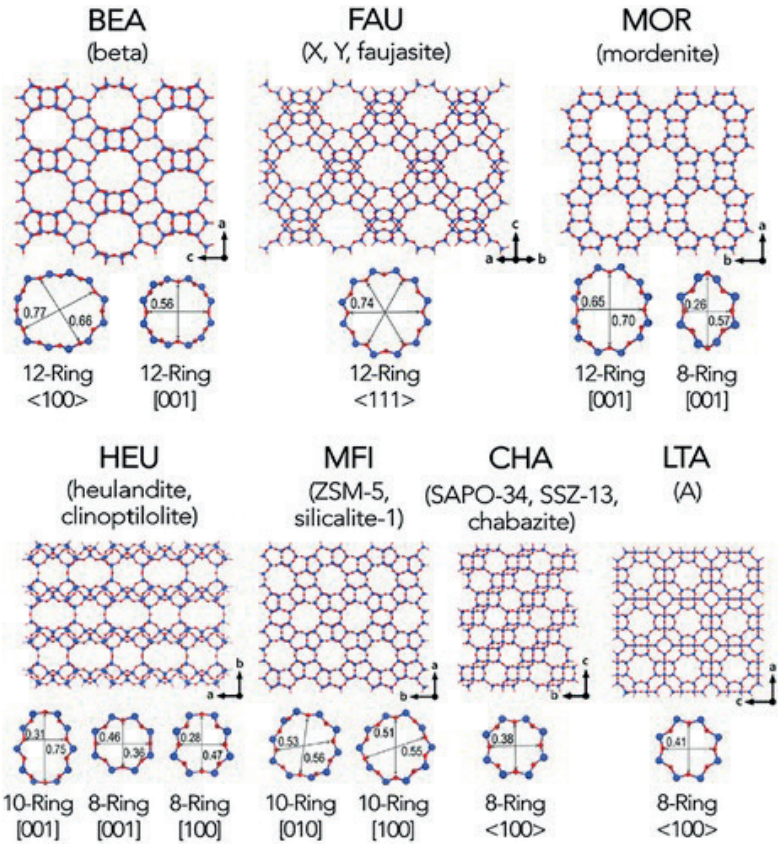


Figure 6.1 Zeolite framework varieties. Red represents O atoms, blue = Si and Al atoms (D. Yang et al., 2021).

(II) Organic framework materials

For a long time, scientists have been interested in studying covalent chemistry (Hassan et al., 2020). Covalent bonds enable MOFs and COFs to form the joint of molecular building pieces, contributing to the accuracy and versatility of covalent science from molecules to more complex organized structures (Hassan et al., 2020) (D. Yang et al., 2021)(Figure 6.2B). Due to varying chemical binding energies between molecular building blocks, these two possibilities exhibit distinct stability and crystallization (J. Liu et al., 2021). They are both crystalline substances with atomically precise porosity framework architectures. Strong covalent linkages give rise to ongoing porosity (Figure 6.2A) in MOFs and COFs structures, making them more robust than some of earlier-developed metal-bipyridine structures made of metal-L base bonds (Kianfar, 2020; D. Yang et al., 2021). This gives MOFs and COFs properties that are comparable to those of conventional porous materials like zeolites. Like their many special qualities, MOFs and COFs have lately been used with remarkable results to catalyze the transformation of biomass platform molecules (Weng et al., 2024).

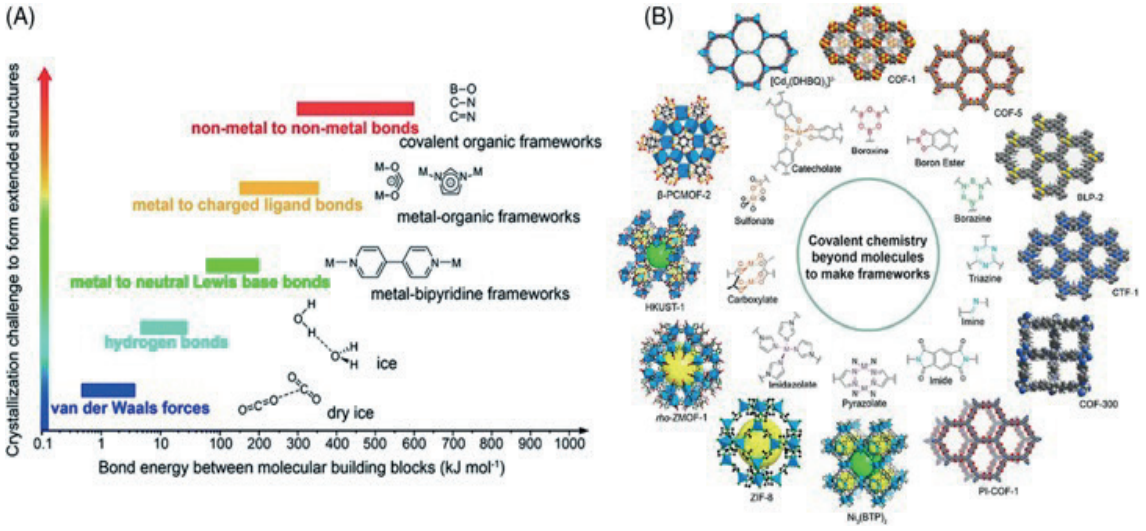


Figure 6.2 (A) The bond energy of the connections between molecule building blocks and the stability and crystallization of crystalline expanded structures are correlated. **(B)** Common COF and MOF kinds with various covalent connections (D. Yang et al., 2021).

(a) Metal–organic framework

Since its initial report by Yaghi's group, MOF—which consists of porous structures formed by metal (nodes) plus organic ligands (linkers) through coordination bonds—has attracted a lot of attention (Du et al., 2022). MOF has customizable morphologies, structures, and physical properties since most transition alloys, post-transition metals, and lanthanides may serve as nodes, and bi- and tri-carboxylate-involved benzene rings and N-involved cycloalkane can be linkers (Iniyan et al., 2023). Over 20,000 different varieties of MOFs have been recorded to far, including ZIF-8, MIL-53, UiO-66, MOF-808, HKUST-1, and others (Al Obeidli et al., 2022). Figure 6.3 displays a few common MOF structures. Furthermore, via ligand exchange and heating post-treatment, MOFs can serve as designs or indicators to form carbons that are porous (PCs), metal-encapsulated PCs, and permeable metal oxide (Chu et al., 2021). This process produces a rapidly growing number of hybrid MOFs and makes it easier for MOFs to be used in a wide range of applications (Chu et al., 2021).

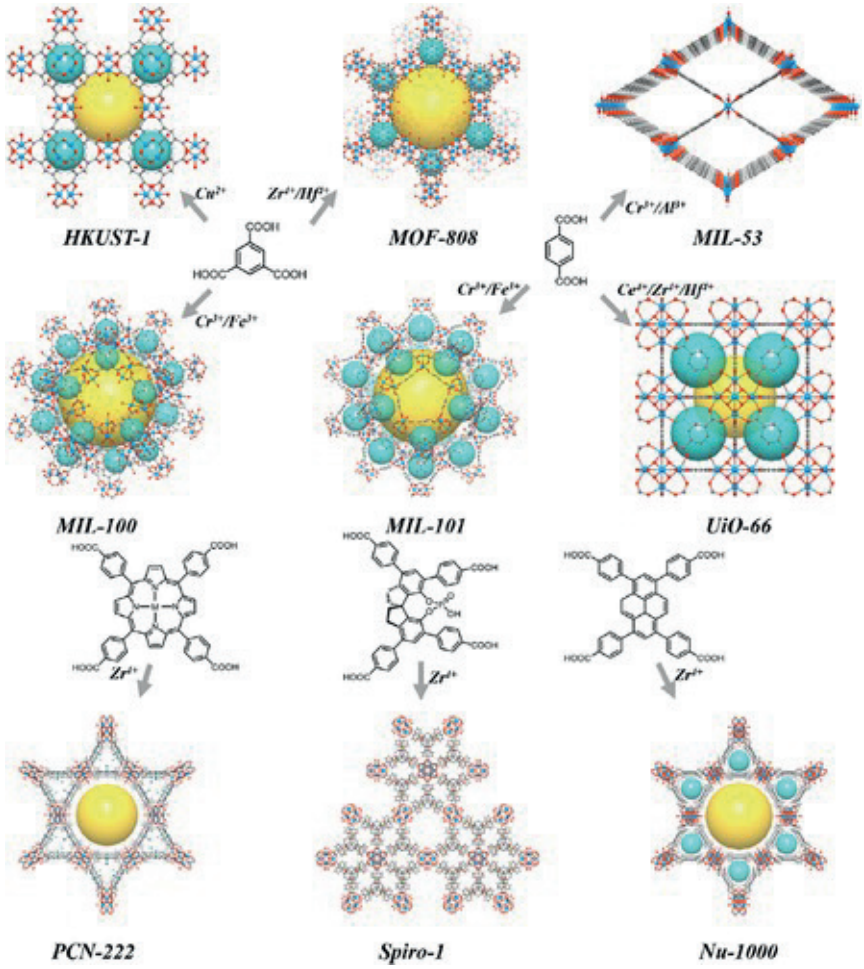


Figure 6.3 Common MOF kinds with various active sites (D. Yang et al., 2021).

(b) Covalent organic framework

Several organic linkers are polymerized to create COF, a natural polymeric component (Figure 6.4). In this instance, COF's crystallinity is reduced because of its more stable structure compared to MOF, which has metal-oxide linkages and a framework connected by strong covalent connections (Gong et al., 2023). Furthermore, the pre-made linker monomers can regulate the spatial architectures of COFs. It has been claimed that a variety of chemical linkers, including sp2-carbon, boroxine, imine, boronic ester, hydrazone, triazine, and phenazine, can produce COFs (Gong et al., 2023). Like MOFs, COFs can also be an excellent platform for modifying materials using a variety of techniques, including chemical conversion, metalation, functionalization, and monomer truncation, to produce a variety of multifunctional materials (Bukhari et al., 2023).

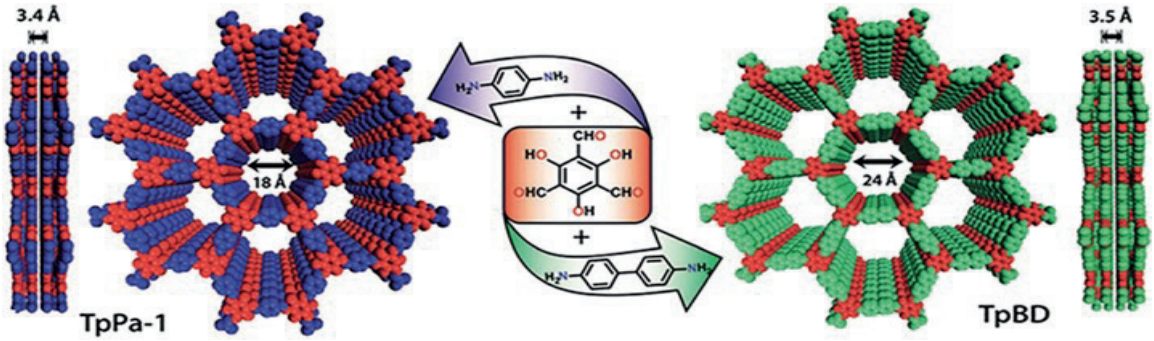


Figure 6.4 Diagrams that show the porous apertures and stacking lengths for the COFs and the packing models during synthesis (D. Yang et al., 2021).

Cluster materials

(I) Polyoxometalate

Polyoxometalate (POM) is a particular type of anionic poly-nuclei metal-oxygen cluster (Lockey et al., 2022). POM generally falls into two categories: heteropolyoxometalates ([XxMyOz]n-, X = Si, P), where negative electrical charge is balanced by counter cations, and isopolyoxometalates ([MxOy]n-, M = V, Mo, W, Nb, Ta, and Ti) (D. Yang et al., 2021). MO6 octahedra, MO5 pentahedra, or MO4 tetrahedra make up most common POM formations (Lockey et al., 2022). Figure 6.5B lists ten types of documented structures, including Lindqvist, Keggin, Anderson, Dawson, and others (D. Yang et al., 2021). Different counter cations, heterometals, ligands, and coordination polyhedral thereby provide POM with varying L/B acid and redox characteristics (Lin, 2021). POM can serve as a great starting point to create a variety of permeable crystal structure materials (Figure 6.5A) (Lin, 2021). Furthermore, POM can be added to specific structural crystalline porous materials, such COF, MOF, and so on, to create novel materials with improved performances in addition to preventing POM from aggregating and deactivating during the catalytic process (Cui & Hu, 2021).

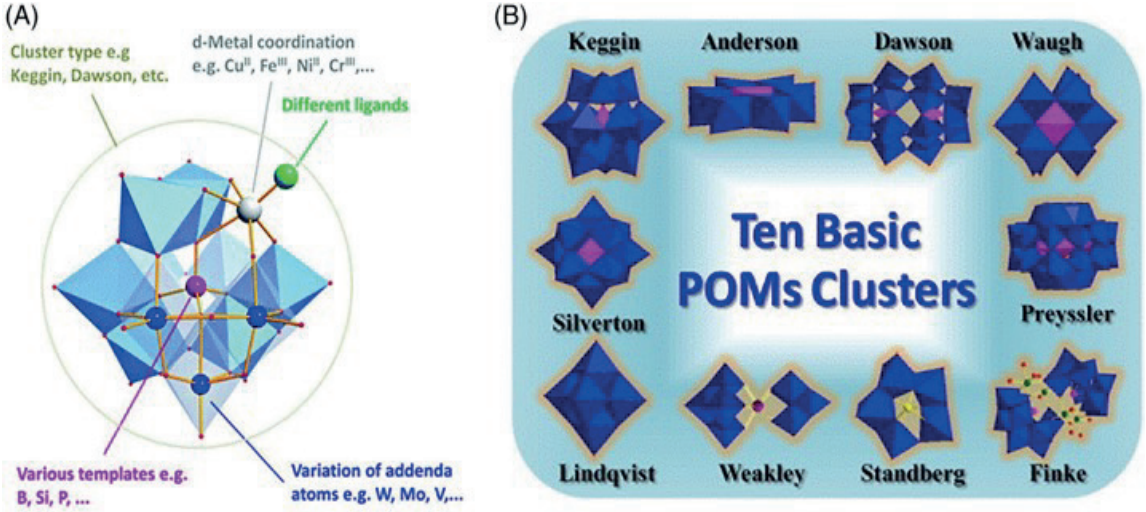


Figure 6.5 (A) Modification sites in polyoxometalate, such as the template, addenda, heterometal, ligand, and counterions; and **(B)** the ten fundamental POM cluster structures (D. Yang et al., 2021).

(II) Metal nanoclusters

Several or even hundreds of metal atoms make up a metal nanocluster, a novel "small" (1 ~ 3 nm) ligand-protected metal nanomaterial that differs from traditional big nanoparticles in that each atom has a distinct energy level (Zhu, 2023) (Maqbool et al., 2023). With surface "staple" structures and kernel structures made up of metal atoms, nanoclusters have their own unique atomic structures. Keep in mind that maintaining the stability of the nanocluster structure depends on the surface structure (Zhu, 2023). Numerous metal nanoclusters have been described up to this point, including mono-metallic Au, Cu, Ag, Ni, Pd, and bi-metallic nanoclusters (Figure 6.6A) (Kang et al., 2020; D. Yang et al., 2021). As an illustration, the gold nanocluster (Figure 6.6B) features a variety of kernel configurations, including face-centered cubic (fcc), body-centered cubic (bcc), hexagonal close-packed (hcp), and icosahedral and biicosahedral structures. Aux (SR)x+1 "staple," such as monomeric staple M-SR-M, dimeric staple SR—AU—SR—AU—SR, pentameric Au5(SR)6, and so on, serve as the main defense for the surface structure (Zou et al., 2023). As a result, metal nanoclusters with clearly defined active sites and high molecular purity can occasionally outperform nanoparticle catalysts, providing platforms for deciphering the atomic-level catalytic mechanism and the structure-catalytic property link (Pei et al., 2024).

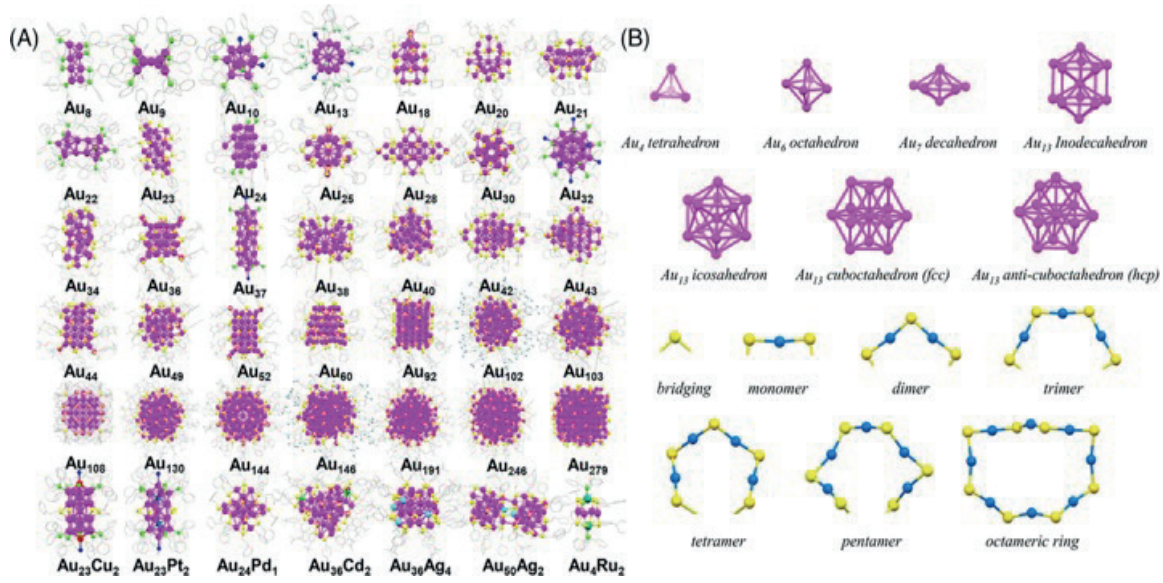


Figure 6.6 (A) Crystal structures of typical Au nanoclusters. **(B)** Au nanoclusters' fundamental kernel architectures and surface-protecting motifs (D. Yang et al., 2021).

7- Catalysis for Sustainable and green Chemistry

Creating catalytic chemical reactions for an environmentally friendly future is an ongoing task spanning several fields of study. Multidisciplinary approaches involving the environment, industry, society, and economic sectors are needed (Cámara et al., 2022). Additionally, to attain increased sustainability, catalytic chemical processes need to be continuously assessed, particularly when used in enterprises or on a household level. Indeed, creating a sustainable future requires chemical catalysis (Sheldon, 2022). Since chemical reactions are used in so many diverse processes, including the production of fuels, food, medicine, and energy, they are inextricably linked to our topic (Lynd et al., 2022).

Here, we incorporate scientific knowledge to assist make these procedures more environmentally friendly. As a result, it lessens the adverse effects on the environment. Reducing the energy required for the processes is essential for chemical catalysis (Lopez et al., 2023). This helps make these systems possible by lowering the usage of energy sources that cause pollution, including fuels sourced from petroleum (Sharma & Shrestha, 2023). Moreover, the increased requirement for high pressure and temperature settings leads to higher energy consumption and, as a result, the generation of waste that contaminates the environment (Kumar et al., 2022). Therefore, the goal of chemical catalysis must be to lower the energy needed for these procedures, such as in the creation of strong catalysts. The development of durable catalysts for use in industry can take various forms, including solid, liquid, or gaseous (Sharma & Shrestha, 2023). The production of desired products must be a part of the catalysts' sustainable working principle. A stabilization power, or the catalyst's ability to be reused in the same process again, reduce the creation of polluting species, and be economically feasible, is another important consideration in the creation of sustainable catalysts (Centi & Perathoner, 2023). Catalytic systems are thus realized on a broad scale through the establishment of sustainable reaction processes. It is possible to lower the amount of energy and environmentally harmful trash produced by using this method. This fact supports green chemical methods and suggests a reduction in the amount of energy derived from oil (Grilli et al., 2023).

Thus, catalysis plays a distinct role in the development of clean, renewable, and ultimately sustainable technology. In this sense, catalysis plays a key role in the creation of fuel cells, which sustainably transform chemical energies into electrical energy (Khademi et al., 2023). Similarly, the process of catalyzing the conversion of biomass—a renewable resource—into biofuels is essential

(Kumar et al., 2022). Today's scientific research enhances the creation of efficient, ecologically friendly, and catalytic chemical processes. Given its attributes, including ease of preparation, low cost, and high catalytic activity, Santos et al. (2023) established prepared WxCeMnOδ/3DOM $ZrTiO_4$ catalysts with usage possibilities for the simultaneous removal of soot particles and oxides of nitrogen from the diesel engine exhaust (Santos et al., 2023). Upon analysis, the produced materials exhibited high levels of structural and catalytic activity. Its flawless structure, plenty of acid sites, sizable area of surface, and the synergistic interaction of the active ingredients all contribute to its high catalytic power. In addition to showing general thermal endurance (250°C–396°C) at the smallest temperature for 90% NO conversion, the produced catalyst W1CeMnOδ/3DOM $ZrTiO_4$ also had an outstanding NO conversion rate (52%) at the soot combustion temperature (Santos et al., 2023).

One ongoing concern is the decrease of greenhouse gas emissions. This information aids in the creation of effective catalytic processors that work together to lessen these impacts. In this regard, Usman et al.'s work offered a suggestion for using catalysts based on Cu, Zn, and Al to catalytically hydrogenate CO2 into useful compounds such methanol (MeOH) and dimethyl ether (DME) (Usman et al., 2023). By using this method, the researchers were able to show how the CO2 and H2 adsorption equilibrium values on the catalysts supplied information on the reaction process. The capacity for adsorption of the reagents was found to relate to the catalytic function, conversion, and yields under investigation. This correlation was confirmed at pressure and temperature that were like those of the hydrogenation reaction. As such, a novel method can be employed to assess and aid in the creation of novel catalysts (Usman et al., 2023). Applications of sustainable catalytic processes can benefit from the use of enzymes (Noor et al., 2022). Because of their distinct catalytic behaviour, enzymes are extensively researched in a variety of catalysis processes. Enzymes can participate in a variety of processes of industrial importance, including alcoholysis, C-C bond formation, transesterification, and esterification (Noor et al., 2022).

Many industrial processes use enzymes, including those in the dairy industry (cheese recovery, flavor improvement, and enzyme-modified cheese (EMC) the manufacturing process), pharmaceutical industry (ibuprofen, naproxen), detergent industry, agricultural industry (pesticides, insects), chemical industry, and oil chemical reactions (fats and oil hydrolysis and bio-detergent synthesis) (Acharya et al., 2022). Because of their unique characteristics, enzymes can be used in place of chemical catalysts in addition to modifying the parameters of the reaction of interest. In this situation, changes to their side chains, domain alterations, and amino acid residues can result in the altering of enzyme activities (Corbella et al., 2023). The function of residue modification on the catalytic function and molecular identification of an alpha-chymotrypsin (CHT) enzyme in the context of a formalin covalent crosslinker was investigated by Biswas et al. in their investigations (Biswas et al., 2022). As the formalin concentration was increased, the results showed a decrease in catalytic activity (Biswas et al.). But the results of (Biswas et al.'s) work might provide insights into drug-target interaction, molecular identification, and macromolecular modification in the future, allowing for the creation of novel binding sites for improved ligand binding via DNA engineering proteins (Biswas et al., 2022).

These days, there is a lot of focus on molecular hydrogen (H2) as the main sustainable fuel for various uses in the future (Ahad et al., 2023). Using catalysts made of precious metals is one method of producing molecular hydrogen (Solakidou et al., 2023). The goal of Kaim et al.'s work was to create substitute non-precious metal catalysts for platinum in the production of hydrogen (Sukackienė et al., 2023). The study employed the enzyme hydrogenase as a model. The variety of elements in a periodic table that are suitable for catalyzing the hydrogen evolution reaction is increased by these investigations with manganese catalysts. Since manganese was included as an extra metal atom that is abundant on Earth in the sequence of mononuclear hydrogen generators, Kaim et al.'s work created a new avenue for research on sustainable hydrogen synthesis. Moreover, manganese is an intriguing option for hydrogen due to its inexpensive cost, wide availability, and

benign environmental profile (Sukackienė et al., 2023).

Gaining a thorough grasp of chemical reactions and optimizing systems requires elucidating the role and catalytic features of enzymes (Taylor et al., 2023). To this end, the latest developments quantum mechanics/molecular mechanics (QM/MM MD) simulation of Born-Oppenheimer was employed in the studies of Liu et al. to systematically understand the mechanism of deAMPylation of AMPylated BiP catalyzed by the enzyme FICD (filamentation induced by cAMP domain protein, commonly referred to as HYPE) (M. Liu et al., 2023). Instead of the common theory that refers to a nucleophilic attack of water molecules adding, the investigations were able to demonstrate that the transfer of protons from the protonated histidine (His363) in FICD to the AMPylated threonine (Thr518) in BiP commences the deAMPylation process. Moreover, it was discovered that humans can change the critical AMPylation inhibitor Glu234—which has been shown to be necessary for the bacterial deAMPylation process (M. Liu et al., 2023). Liu et al.'s study clarifies the physiological function of the FICD protein and posttranslational modifications (PTMs).

8- Catalytic Applications in Energy Conversion

A key force in the energy countryside, catalysis affects processes all the way through the energy life cycle (Hosseinzadeh-Bandbafha et al., 2023). Catalytic processes are crucial in determining how energy systems are shaped, from the conventional production of fossil fuels to the emergence of environmentally friendly energy sources like hydrogen energy and artificial photosynthesis. The complexity of catalysis in energy applications is explored in this chapter, which presents studies and reviews that provide insight on the complex interplay between catalytic mechanisms and the changing energy paradigm (Afolabi, 2024). Catalytic processes play a major role in traditional fossil fuel extraction by allowing hydrocarbons to be valuably extracted. In this situation, catalytic reaction optimization is still crucial for efficiency and environmental reasons catalysis plays a key role in enabling greener and more sustainable energy alternatives, such as the generation of biofuel from renewable resources or the removal of CO_2 from the environment from power plants, or industrial sites (S. Li et al., 2023).

The move to sustainable energy brings with it new opportunities and problems, and catalysis turns out to be a major facilitator of this change (Isahak & Al-Amiery, 2024). One major area of focus is hydrogen as a green energy carrier. The creation, storage, and use of hydrogen depend heavily on catalysis, which also affects the feasibility and efficiency of hydrogen as an environmentally friendly fuel (Muhammed et al., 2023). Solar light-harvesting systems have gained significance in the quest for renewable energy (Bouclé et al., 2023). In these efforts, catalysis plays a crucial role, especially in the creation of materials and procedures for artificial photosynthesis. These developments hold potential for sustainable energy generation since they mimic nature's efficiency in absorbing and transforming solar energy into chemical energy.

Anwar et al. presents a novel electrocatalyst made by pyrolyzing Cu-tpa MOF with low Pt loading and exhibits good ORR performance on par with commercial Pt/C (Anwar et al., 2020). It is highlighted that metal-organic frameworks (MOFs) can be used as precursors for nanocomposites because of their stable electrochemical reactions at elevated temperatures and distinct porosity architectures. Using density functional theory (DFT) computations to improve our understanding of ORR catalysis is another important issue (Liao et al., 2022). The effect of CO_2 activation and reduction on faulty FeS surfaces is thoroughly investigated by Dzade et al. Having such mechanistic insights is crucial to creating effective CO_2 conversion catalysts (Dzade & de Leeuw, 2021).

Moreover, the papers devoted to coordination compound-derived and perovskite-based catalysts demonstrate creative methods for overcoming ORR-related difficulties. A highly effective and long-lasting LaMnO3@C-Co_3O_4 composite is introduced in the study by Karuppiah, et al. which shows excellent oxygen electrocatalysis in an alkaline environment (Karuppiah et al., 2021). Expanding on the thoughtful contributions previously mentioned, a variety of further groundbreaking

discoveries that push the boundaries of catalysis for uses in energy. A simultaneous electrocatalyst for the oxygen reduction process (ORR) is introduced by Sridharan et al. In alkaline media, the combination of Co-doped CeO2 and N- and S-doped reduced graphene oxide (rGO) showed improved ORR performance. By highlighting the possible uses of the synthesized electrocatalyst beyond conventional fuel cells and metal-air batteries, this study highlights its versatility (Sridharan et al., 2022).

An interesting reversal of the photo galvanic effect caused by doping NiSalen polymers with anionic porphyrins is explored in the article by Petrov et al. This surprising occurrence presents a new facet in the field of photoelectrochemical processes and opens new paths for studying the interaction between conductive polymers and dopants. It was investigated using ultraviolet-visible spectroscopy and cyclic voltammetry (Petrov et al., 2021). In addition, Cross et al. offer a basic knowledge of Ni3N surfaces related to the hydrogen evolution reaction (HER). The study provides knowledge about the durability of Ni3N surfaces, water adsorption, and energies of activation for HER using dispersion-corrected density functional theory (DFT-D3). This thorough theoretical approach provides important insights for designing effective Ni-based HER catalysts (Cross et al., 2021).

Aladeemy et al. discuss the electrooxidation of urea, a vital step in the treatment of wastewater. When nickel hydroxide was electrodeposited onto commercial carbon paper using dimethyl sulphoxide solvent, an extremely stable and active electrocatalyst for the electrooxidation of urea in an alkaline environment was produced. This work presents a viable method using transition metal electrocatalysts to activate commercial carbon paper (Aladeemy et al., 2021). Furthermore, Matienzo et al. assess perovskite materials for alkaline water electrolysis's oxygen revolution reaction (OER). To provide a methodical evaluation of perovskite-based electrocatalysts for sustainable energy production, the study considers industry requirements and criteria (Matienzo et al., 2020).

A novel method is used by Alekseeva et al. to create a bimetallic Cu/Pt catalyst. This product demonstrated exceptional resistance to the existence of methanol in the solution in addition to having significant activity in the ORR. The continuous efforts to create effective catalysts for fuel cell applications are aided by this work. The wide variety of catalysts investigated and the use of sophisticated methods like DFT calculations not only expand our knowledge but also create opportunities for the creation of more sustainable and effective energy conversion systems (Alekseeva et al., 2020).

9- Emerging Trends and Future Directions

In the past, transition metal catalysts have dominated the area of catalysis in chemistry. Precious metals have been essential in creating catalysts for novel processes of chemical bonding activation and creation because of their special set of features (Vieira et al., 2023). However, one significant and inherent disadvantage of precious metals is their scarcity; developing alternate catalysis mechanisms is important factor in modern research to shift chemistry to more environmentally friendly utilization of the world's scarce resources. One of the most important contributions to solving the most pressing global issues is heterogeneous catalysis (Low et al., 2023). The common characterization methods and ideas in the most recent literature represent a trend that the catalysis field has seen in recent years: a blurring of the lines separating traditional thermal catalysis, photocatalysis, and electrocatalysis (Suremann et al., 2023).

Three main topics may be identified in the current state of catalysis research: the creation of novel catalysts, the investigation of reaction mechanisms, and reaction design for specific processes (Zhao et al., 2023). In catalysis research, creating catalysts with novel structures or formulations might always encourage the study of new phenomena. From a fundamental perspective, comprehending the molecular and atomic arrangements of solid catalysts is essential for designing catalytic materials logically and for desired reactions (S. Xu et al., 2024). The manner of contemporary research on

catalysis reflects this tendency, typically utilizing numerous advanced characterization techniques to disclose the atomic and molecular structures of the active sites. Practically, advances in materials fabrication and reaction engineering have demonstrated significant promise in tackling global issues like climate change and the switch from fossil fuels to clean energy sources (Kar et al., 2024).

Future catalyst development is anticipated to focus on two primary areas: developing new processes that make use of different raw materials with the help of new catalysts and refining current methods to increase yield and selectivity while saving energy in the production process (Serrano et al., 2024). Homogeneous transition metal catalysis is currently essential to the wide range of catalytic processes and is predicted to become even more important in the future.

In homogeneous catalysis, data-driven knowledge development based on premium databases and machine learning algorithms is revolutionizing the profession (H. Li et al., 2023). Catalytic transformations have traditionally been developed or improved using computational mechanistic studies or trial and error methods. On the other hand, new experimental and digital methods are generating catalytic system data more quickly, which makes it easier to train predictive machine learning models for catalyst discovery (Mace et al., 2024). Notwithstanding the encouraging developments in the subject, several problems, including a lack of data and code transparency, are impeding the industry's advancement. For that reason, we believe that to fully utilize ML approaches, an open access philosophy about methods and data will be essential (Casacuberta et al., 2024). Furthermore, we believe that easily navigable interfaces like ROBERT and public repositories like the ioChem-BD database will be critical in facilitating the wider chemistry community's adoption of machine learning (ML) tools and bringing them closer to organic/organometallic laboratories in near future (Tom et al., 2024).

10- Challenges and Opportunities in Catalysis

Catalyst innovation has led to numerous advancements in industrial chemistry, and it is possible that catalysts will hold the key to solving today's problems. Scholars have discovered new applications for catalysts to address issues in business, health, and the environment. These investigations could grow into large-scale applications in the upcoming years.

10.1 Machine Learning

Since novel catalysts are often extremely complicated structures with a wide range of features, designing them has consistently been a trial-and-error process. Because of this intricacy, researchers find it very challenging to forecast the effects of minute modifications to the structure on performance. They must instead rely on real-world trials of every variant, which adds cost and time to the research process by creating, testing, and then discarding many potential outcomes.

However, a fresh method for designing catalysts is provided by developments in machine learning (Zhuang et al., 2024). Catalysis research is only one of several sectors using artificial intelligence (AI) to tackle problems as machine learning advances. In ways that humans could never notice, specially trained programmers are able to use extra data to make predictions and identify patterns and correlations. Machine learning can save time and money by reducing the number of possible designs without the need for real-world testing in the catalysis process (Çıtmacı et al., 2022).

Recently, Chinese researchers showed how machine learning could be applied to catalysis research (Lee et al., 2024). The group's goal was to create a perovskite oxide catalyst that would accelerate oxide reduction in solid-oxide fuel cells through their research on these fuel cells. They might utilize the AI to discover relationships between specific important characteristics and catalyst performance after training it with a carefully chosen data set. By using this approach, the researchers expect to expedite the production of catalysts soon for similar initiatives (Lee et al., 2024).

10.2 Enzyme Engineering

Enzyme engineering has also made use of machine learning. Since enzymes are biological catalysts, businesses have been designing enzymes through genetic engineering. Microorganisms can create enzymes that catalyze processes by modifying amino acids (Porras-Dominguez et al., 2024). Enzyme engineering is a relatively new technique but is already used in industrial and medical operations. Enzyme engineering is not without restrictions, though (J. Yang et al., 2024). Gene manipulation can be an uncertain procedure, and naturally occurring enzymes are typically less robust than modified enzymes. Although some enzyme compositions have eluded scientists, machine learning may be able to change this. Recently, Moderna has created a technique that uses machine learning to improve medicinal enzyme engineering. This method might be modified for industrial application, opening new possibilities for biological catalysis (Feng et al., 2024).

10.3 Alternatives to Precious Metals

Precious metals are catalysts in numerous chemical reactions. Platinum is used in catalytic converters, which is a clear example, but precious metals are also needed in numerous manufacturing processes to catalyze reactions (Willner, 2024). This is obviously a concern because as the supply of these metals decreases and new applications are discovered, the demand will only rise, making them more expensive and difficult to find. In the future, this will pose a significant obstacle to catalysis, so scientists are already looking for a substitute. Though progress is sluggish, some strides have been made.

Photocatalysis has been found to be an effective substitute for precious metal catalysts in some reactions, according to research conducted in conjunction with Princeton University, Rice University, and Syzygy Plasmonic Inc. (H. Li et al., 2024). Light can accelerate catalysts known as photocatalysts because photon energy excites electrons and produces free radicals (Jiang et al., 2023). Though photocatalysts have been theoretically proposed for almost a century, commercial applications have not yet been realized.

In this project, ammonia was converted to hydrogen for use in fuel cells using a photocatalyst based on iron (G. Li et al., 2023). Previously, ruthenium—much harder to get than iron—was employed in this reaction. The accomplishments of this group are noteworthy for precious metal catalysis in general as well as for this particular technique. It moves the industry closer to creating photo catalysis and displacing precious metals. In this project, ammonia was converted to hydrogen for use in fuel cells using a photocatalyst based on iron. Previously, ruthenium—much harder to get than iron—was employed in this reaction. The accomplishments of this group are noteworthy for precious metal catalysis in general as well as for this particular technique. It moves the industry closer to creating photo catalysis and displacing precious metals (G. Li et al., 2023).

10.4 Electro catalysis

Catalysts employed in electrochemical reactions—those brought on by an electric current—are known as electrocatalysts (Toan et al., 2023). Electrocatalysts are already used in a lot of electrochemical processes, but scientists are working to make them more robust and effective. Fuel cells made of hydrogen are one application for them. Fuel cells aren't a reliable source of energy since the electrochemical process of separating hydrogen and oxygen molecules takes too much energy now (Christopher & Dimitrios, 2012). Electrocatalysts with higher efficiencies have been researched for decades with the goal of developing fuel cell technology. Because it would address the problem of energy storage, this would be a huge advancement for green energy (G. Zhang et al., 2024).

10. 5 Catalytic Waste Management

Catalysts may be the answer to tackling another environmental problem, namely plastic

waste. It is commonly known that plastic is difficult to dispose of due to its extraordinarily extended breakdown time (Dey et al., 2024). Existing techniques, like mechanical recycling, incineration, and landfills, all have serious disadvantages, and attempts to cut back on plastic use have failed because garbage output keeps rising. Some researchers are using catalysis to stop this epidemic of plastic trash (Yim et al., 2024). Several investigations have discovered catalysis-based techniques for handling different types of polymers (Naumann, 2023). These techniques not only reduce waste but also yield useful goods like chemicals or fuel that can be put back to use in other industrial processes. This warrants funding for such technologies from an economic and from an environmental perspective.

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