STM JOURNALS

Journal of
Catalyst & Catalysis

ISSN: 2349-4344
Volume 13, Issue 2, 2026
May–August
DOI (Journal): 10.37591/JoCC

http://engineeringjournals.stmjournals.in/index.php/JoCC/index

Review JoCC

Integrated Computational and Bio-catalytic Transformations: DFT-Guided Mechanistic Insights, Machine Learning, and Nano-biocatalyst Engineering for Sustainable Catalysis

Sandeep Rai

Abstract

Computational catalysis has emerged as a transformative scientific discipline that integrates quantum chemistry, molecular modeling, machine learning, and density functional theory (DFT) to understand catalytic mechanisms and design highly efficient catalytic systems for sustainable industrial applications. The increasing global demand for environmentally responsible chemical manufacturing has accelerated research on advanced catalytic materials including transition metal catalysts, metal–organic frameworks (MOFs), homogeneous catalysts, heterogeneous systems, and bimetallic catalysts involving nickel and iron. These catalytic systems play a significant role in hydrogenation, methanation, carbon dioxide conversion, and carbon–carbon bond formation reactions. Computational chemistry provides atomistic-level insights into adsorption behavior, electronic structures, catalyst stability, and activation energy barriers, thereby enabling rational catalyst optimization before experimental synthesis. Recent computational studies have provided detailed mechanistic understanding of elementary reaction steps such as oxidative addition, transmetallation, ligand exchange, and reductive elimination in cross-coupling chemistry. DFT-based approaches have enabled accurate prediction of catalytic activity, reaction energetics, scaling relations, adsorption energies, and volcano plots for methanation reactions and catalytic carbon–carbon coupling processes. Machine learning and artificial intelligence have further accelerated catalyst discovery by identifying nonlinear relationships between catalyst descriptors and catalytic performance, thereby reducing the need for extensive trial-and-error experimentation. In parallel, biocatalytic transformations using immobilized enzymes, engineered proteins, and nanobiocatalysts have gained increasing importance for environmentally friendly synthesis under mild operating conditions. Nanostructured supports, multifunctional hybrid catalytic systems, and enzyme immobilization technologies have improved catalytic stability, selectivity, and reusability for industrial biotechnology applications. This paper discusses recent advances in computational catalysis and biocatalytic transformation with emphasis on mechanistic understanding, catalyst engineering, green nanomaterials, process intensification, and sustainable industrial applications in energy, pharmaceuticals, environmental remediation, and fine chemical synthesis.

*Author for Correspondence
Sandeep Rai
E-mail: sadeep1964@yahoo.co.in,

DPC Member, Department of Chemistry, UPL University of Sustainable Technology, Block No. 402, Ankleshwar-Valia Road, Taluka: Valia, Dist.: Bharuch, India

Received Date: June 02, 2026
Accepted Date: June 11, 2026
Published Date: June 25, 2026

Citation: Sandeep Rai. Integrated Computational and Bio-catalytic Transformations: DFT-Guided Mechanistic Insights, Machine Learning, and Nano-biocatalyst Engineering for Sustainable Catalysis. Journal of Catalyst & Catalysis. 2026; 13(2): 36–44p.

Keywords: Computational catalysis, Density functional theory, Machine learning, Nickel catalyst, Iron catalyst, Methanation, Nanobiocatalyst, Enzyme immobilization, Green chemistry, Transition states

INTRODUCTION

Catalysis plays a central role in modern chemical manufacturing, environmental remediation, and energy conversion technologies. A significant proportion of industrial chemical processes depend on catalytic systems to improve reaction rates, enhance selectivity, and reduce energy consumption. In recent decades, computational catalysis has emerged as a powerful scientific approach for understanding catalytic reactions at atomic and molecular levels. The rapid development of advanced quantum chemistry methods, particularly density functional theory (DFT), has revolutionized the investigation of catalytic systems by enabling prediction of reaction pathways, adsorption energies, activation barriers, electronic structures, and transition states with high accuracy. Computational chemistry is now extensively applied to heterogeneous catalysis, homogeneous catalysis, organometallic chemistry, and metal–organic frameworks (MOFs) for industrially important transformations including hydrogenation, methanation, carbon dioxide reduction, and carbon–carbon bond formation reactions [1].

Computational approaches provide detailed mechanistic insights into elementary reaction steps such as oxidative addition, transmetallation, ligand exchange, surface adsorption, and reductive elimination. These studies enable rational catalyst design and optimization prior to experimental synthesis, thereby reducing material costs, energy consumption, and experimental effort. Transition metal catalysts based on nickel, iron, palladium, and cobalt are widely investigated because of their importance in sustainable chemical manufacturing and renewable energy technologies. In particular, nickel- and iron-based catalytic systems have gained attention as low-cost and environmentally friendly alternatives to noble metal catalysts for methanation, hydrogenation, and environmental catalytic applications.

The integration of machine learning and artificial intelligence into catalytic research has further accelerated catalyst discovery and optimization. Machine learning models trained on DFT-generated datasets can identify structure–activity relationships, predict adsorption energies, classify catalytic behavior, and estimate reaction kinetics with remarkable efficiency. Descriptor-based modeling, scaling relations, and volcano plot analyses have become important computational tools for evaluating catalytic performance and screening large numbers of catalytic materials. Such computational approaches are especially important in methanation reactions, carbon dioxide utilization, electrochemical energy conversion, and transition metal-mediated cross-coupling chemistry [2].

Alongside computational catalysis, biocatalysis has gained considerable prominence because of its exceptional selectivity, mild operating conditions, biodegradability, and environmental compatibility. Enzymatic catalytic systems are increasingly employed in pharmaceutical synthesis, food processing, biofuel production, and environmental remediation. Advances in enzyme immobilization, protein engineering, nanobiocatalysts, and multi-enzymatic cascade systems have significantly improved catalytic stability, reusability, and industrial applicability. Nanostructured supports and multifunctional hybrid catalytic systems further enhance catalytic performance and process efficiency for sustainable chemical manufacturing.

The convergence of computational chemistry with biocatalytic engineering represents a promising pathway toward environmentally responsible and economically viable chemical technology. Computational tools enable detailed understanding of enzyme mechanisms, substrate interactions, and catalytic pathways, thereby supporting rational biocatalyst optimization. Simultaneously, process intensification strategies, continuous-flow bioreactors, and hybrid chemoenzymatic systems contribute to greener and more energy-efficient industrial processes. This paper reviews recent developments in computational catalysis and biocatalytic transformation with emphasis on catalyst design, mechanistic understanding, machine learning-assisted optimization, enzyme engineering, nanobiocatalysts, and sustainable industrial applications [3].

QUANTUM CHEMISTRY AND DENSITY FUNCTIONAL THEORY IN CATALYSIS

Quantum chemistry provides the theoretical foundation for studying catalytic reactions at the electronic and molecular levels. Modern computational approaches enable detailed understanding of catalyst structures, adsorption behavior, bond activation, and elementary reaction mechanisms. Among available computational techniques, density functional theory (DFT) has become the most widely used approach because it offers an effective balance between computational cost and predictive accuracy.

DFT calculations allow investigation of catalytic pathways, activation barriers, transition states, and electronic interactions in heterogeneous and homogeneous catalytic systems. These methods are now extensively applied in transition metal catalysis, metal–organic frameworks (MOFs), methanation chemistry, and carbon–carbon bond formation reactions.

Density Functional Theory and Transition States

DFT calculations are commonly employed to identify reaction intermediates, transition states, adsorption energies, and activation barriers in catalytic systems. Transition-state theory enables prediction of reaction kinetics and determination of rate-determining steps in catalytic cycles. Computational studies provide atomistic insight into elementary transformations including oxidative addition, transmetallation, ligand exchange, and reductive elimination in transition-metal-catalyzed cross-coupling reactions. Such mechanistic understanding is essential for catalyst optimization and rational design of efficient catalytic systems.

For nickel-catalyzed alkyl–alkyl Negishi cross-coupling reactions, computational investigations have demonstrated that oxidative addition frequently proceeds through single-electron transfer pathways involving radical intermediates. Nickel complexes exhibit flexible oxidation states that stabilize multiple reaction intermediates and facilitate radical-mediated catalytic mechanisms. DFT calculations reveal that ligand properties strongly influence activation barriers, catalyst stability, electronic distribution, and selectivity. Electron-rich ligands generally stabilize low-valent nickel species, while sterically demanding ligands influence transition-state geometries and reaction energetics. These studies have significantly improved mechanistic understanding of nickel-mediated catalytic cycles [4].

Ligand Effects and Catalytic Selectivity

Ligands play a crucial role in controlling catalytic activity, selectivity, and stability in homogeneous catalysis. Steric and electronic effects modify the coordination environment of transition metals and directly influence adsorption energies, transition-state structures, and catalytic pathways. Computational chemistry enables prediction of ligand-dependent reactivity trends and provides mechanistic insights into catalyst performance under varying reaction conditions.

Phosphine ligands containing electron-donating substituents stabilize low-valent nickel species and facilitate oxidative addition processes by increasing electron density at the metal center. Bulky ligands can accelerate reductive elimination through destabilization of sterically crowded intermediates and modification of transition-state geometries. Computational investigations of N-heterocyclic carbenes, bipyridine ligands, and pincer ligands further demonstrate the importance of ligand design in catalyst optimization. Such studies provide valuable guidance for rational development of highly selective and efficient catalytic systems for fine chemical synthesis and industrial transformations [5].

Scaling Relations and Volcano Plots

Scaling relations are important computational tools in heterogeneous catalysis because they correlate adsorption energies of reaction intermediates on catalyst surfaces. These relationships provide simplified models for evaluating catalytic activity and identifying key descriptors that control catalytic performance. Volcano plots generated from scaling relations enable prediction of optimal catalytic activity by identifying balanced adsorption strengths for reactants and intermediates.

Nickel- and iron-based catalysts are extensively studied for methanation reactions and carbon dioxide conversion processes. DFT calculations reveal that adsorption energies of carbon monoxide, hydrogen, and carbon-containing intermediates strongly influence catalytic performance and reaction kinetics. Catalysts exhibiting excessively strong adsorption may suffer from catalyst poisoning and slow product desorption, whereas weak adsorption leads to insufficient activation of reactants. Volcano plot analysis therefore identifies optimal catalyst compositions capable of balancing adsorption and desorption processes for maximum catalytic efficiency [6].

COMPUTATIONAL MODELING OF METHANATION CATALYSTS

Methanation reactions are highly important for synthetic natural gas production, renewable energy storage, and carbon dioxide utilization technologies. Computational chemistry has significantly contributed to mechanistic understanding and catalyst optimization for methanation processes. Nickel-based catalysts remain industrially dominant because of their relatively low cost, high catalytic activity, and favorable selectivity toward methane production.

Nickel Catalysts for Methanation

DFT studies indicate that nickel surfaces activate carbon dioxide through dissociative pathways involving carbon monoxide intermediates and surface-bound hydrogen species. Sequential surface hydrogenation reactions ultimately lead to methane formation. Transition-state calculations reveal that carbon–oxygen bond cleavage is frequently the rate-determining step in methanation reactions. Adsorption energies, surface morphology, catalyst supports, and metal dispersion strongly affect catalytic activity and selectivity.

Bimetallic catalytic systems combining nickel with iron or cobalt often exhibit improved catalyst stability, thermal resistance, and reduced coke formation. Computational models demonstrate that iron incorporation modifies the electronic structure of nickel surfaces and changes adsorption energies of reaction intermediates. Such modifications improve catalytic efficiency and enhance resistance to catalyst deactivation under industrial operating conditions [7].

Metal–Organic Frameworks in Catalysis

Metal–organic frameworks (MOFs) possess exceptionally high surface areas, tunable pore structures, and adjustable chemical functionalities, making them attractive materials for catalytic applications. MOFs are increasingly investigated as catalysts, catalyst supports, and adsorption materials for gas separation and carbon capture technologies. Computational chemistry enables prediction of gas adsorption behavior, diffusion pathways, catalytic activity, and host–guest interactions within porous MOF structures.

DFT investigations of MOF-supported nickel catalysts demonstrate enhanced carbon dioxide adsorption, improved reactant accessibility, and superior catalytic selectivity compared with conventional catalyst supports. Molecular simulations further provide insight into pore diffusion, adsorption thermodynamics, and framework stability. Machine learning approaches integrated with molecular modeling are now widely applied for screening thousands of MOF structures for catalytic and environmental applications [8].

MACHINE LEARNING IN COMPUTATIONAL CATALYSIS

Machine learning has emerged as a highly effective tool for accelerating catalyst discovery and computational screening. Traditional computational methods often require extensive and time-consuming calculations, whereas machine learning approaches significantly reduce computational cost while maintaining predictive capability. Integration of artificial intelligence with computational chemistry is transforming catalyst design and optimization strategies.

Data-Driven Catalyst Design

Machine learning models utilize descriptors such as adsorption energies, d-band centers, coordination numbers, electronic structures, and geometric parameters to predict catalytic performance. Neural networks, random forest algorithms, support vector machines, and regression-based approaches are commonly employed in catalysis research for catalyst classification and property prediction.

For methanation catalysts, machine learning models trained on DFT-generated datasets can predict turnover frequencies, activation energies, selectivity, and catalyst stability. Such approaches enable rapid screening of catalyst libraries and identification of promising catalytic materials prior to experimental validation. Data-driven computational strategies therefore contribute significantly to efficient catalyst discovery and sustainable industrial process development [9].

Interpolation Concepts in Catalyst Discovery

Interpolation methods are highly important in machine learning-assisted catalyst design because they enable prediction of catalytic properties for compositions that have not been explicitly calculated or experimentally studied. This approach is particularly valuable for multicomponent bimetallic and alloy catalysts where the compositional design space is extremely large.

By combining interpolation techniques with extensive DFT datasets, researchers can estimate adsorption energies, activation barriers, and reaction energetics across broad compositional ranges. These computational strategies accelerate identification of optimal catalytic materials and reduce the need for exhaustive quantum chemical calculations. Interpolation-based models therefore support rapid exploration of catalytic composition–property relationships for sustainable catalysis research.

MECHANISTIC STUDIES IN CROSS-COUPLING REACTIONS

Cross-coupling reactions are among the most important transformations in modern organic synthesis because they enable efficient formation of carbon–carbon bonds. Transition-metal-catalyzed cross-coupling processes are extensively applied in pharmaceutical synthesis, polymer chemistry, agrochemicals, and fine chemical manufacturing [10].

Oxidative Addition

Oxidative addition is often the first elementary step in transition-metal-catalyzed cross-coupling reactions. In nickel-catalyzed systems, oxidative addition may proceed through either concerted mechanisms or radical-mediated single-electron pathways depending on ligand structure, substrate type, and reaction conditions. DFT calculations are extensively used to identify energetically favorable reaction pathways and characterize transition states associated with oxidative addition processes.

Transmetallation

Transmetallation involves transfer of an organic group from one metal center to another during catalytic cycles. Computational studies indicate that solvent effects, ligand coordination, and electronic interactions significantly influence transmetallation kinetics and thermodynamics. Understanding these factors is essential for optimizing catalyst efficiency and improving reaction selectivity in cross-coupling chemistry.

Reductive Elimination

Reductive elimination represents the final carbon–carbon bond-forming step that regenerates the active catalyst species. Ligand geometry, electronic structure, steric effects, and coordination environment strongly affect reductive elimination barriers. Computational chemistry provides detailed mechanistic insight into these processes and supports rational catalyst optimization for efficient and selective bond formation reactions.

NMR SPECTROSCOPY AND ISOTOPE LABELING STUDIES

Experimental validation remains essential for confirming computational predictions and establishing reliable mechanistic understanding in catalysis research. Nuclear magnetic resonance (NMR) spectroscopy and isotope labeling experiments are widely employed to investigate catalytic intermediates, ligand environments, and reaction pathways.

NMR spectroscopy enables identification of transient catalytic species, coordination geometries, and dynamic molecular interactions during catalytic cycles. Isotope labeling studies provide valuable mechanistic information regarding bond activation processes, atom transfer pathways, and rate-determining steps. Combined computational and spectroscopic investigations therefore provide comprehensive understanding of catalytic mechanisms and improve reliability of theoretical predictions in computational catalysis research.

BIOCATALYTIC TRANSFORMATIONS AND NANOBIOCATALYSTS

Biocatalysis has emerged as an environmentally sustainable alternative to conventional chemical synthesis because enzymatic reactions operate under mild conditions and exhibit remarkable substrate specificity and catalytic selectivity. Enzyme-based catalytic systems reduce energy consumption, minimize hazardous waste generation, and support green chemistry principles. Advances in nanotechnology, protein engineering, and computational modeling have significantly improved the stability, efficiency, and industrial applicability of biocatalytic systems.

Enzyme Immobilization

Immobilized enzymes exhibit improved operational stability, enhanced reusability, and greater resistance to harsh chemical and thermal conditions compared with free enzymes. Immobilization also facilitates catalyst recovery and continuous processing in industrial applications. Common immobilization methods include adsorption, covalent binding, encapsulation, entrapment, and cross-linking techniques. The choice of immobilization strategy strongly influences catalytic efficiency, substrate accessibility, and enzyme stability.

Nanomaterials such as carbon nanotubes, graphene oxide, mesoporous silica, and magnetic nanoparticles are widely employed as enzyme supports because of their high surface area, excellent mechanical stability, and tunable surface properties. Immobilized enzymatic systems are increasingly applied in pharmaceutical synthesis, food processing, wastewater treatment, biosensing, and environmental remediation. Computational modeling further assists in optimizing enzyme orientation, substrate diffusion, and support–enzyme interactions for enhanced catalytic performance.

Nanobiocatalysts and Green Nanomaterials

Nanobiocatalysts integrate nanotechnology with biocatalysis to produce highly efficient catalytic systems with improved stability and activity. Green nanomaterials synthesized from renewable and environmentally benign resources are increasingly investigated because they reduce environmental impact while maintaining desirable catalytic properties. These materials exhibit enhanced surface interactions, electron transfer capabilities, and catalytic efficiencies suitable for sustainable industrial processes.

Carbon dots have emerged as promising nanomaterials because of their fluorescence characteristics, excellent biocompatibility, chemical stability, and catalytic behavior. Functionalized carbon-dot systems are widely investigated for biosensing, bioimaging, photocatalysis, and catalytic transformation applications. Dual-responsive carbon-dot systems sensitive to pH and hydrogen peroxide are particularly important in biomedical diagnostics and environmental monitoring. Integration of carbon dots with enzymes and metal nanoparticles further enhances catalytic performance and multifunctional applications.

Multi-Enzymatic Systems

Multi-enzymatic systems enable cascade reactions to occur within a single reactor environment, thereby mimicking natural biological pathways and significantly improving process efficiency. Such systems eliminate the need for intermediate purification steps, reduce solvent consumption, and enhance overall reaction selectivity. Multi-enzyme reactors therefore represent an important strategy for sustainable and economically efficient industrial bioprocesses.

Applications of multi-enzymatic systems include nucleoside synthesis, glycosylation, halogenation, acylation, deamination, selective oxidation, and pharmaceutical intermediate production. Immobilization of multiple enzymes on nanostructured supports improves catalytic stability, substrate channeling, and reaction coordination between sequential enzymatic steps. Computational modeling also contributes to optimization of enzyme compatibility, reaction kinetics, and substrate transport within cascade systems.

CARBONIC ANHYDRASE AND INDUSTRIAL APPLICATIONS

Carbonic anhydrase is an important metalloenzyme that catalyzes the rapid hydration of carbon dioxide into bicarbonate ions and protons. Because of its exceptionally high catalytic efficiency, carbonic anhydrase has attracted considerable attention for carbon dioxide capture and conversion technologies aimed at reducing greenhouse gas emissions and supporting sustainable industrial operations.

Computational modeling, molecular dynamics simulations, and enzyme engineering have significantly improved understanding of carbonic anhydrase catalytic mechanisms, active-site interactions, and proton transfer pathways. Immobilized carbonic anhydrase systems are increasingly integrated into membrane reactors, absorption units, and bioreactors for industrial carbon capture technologies. Computational approaches further assist in designing enzyme variants with improved thermal stability, solvent tolerance, catalytic efficiency, and operational durability under industrial conditions. Such developments support the implementation of environmentally friendly carbon management technologies.

BIOPROCESS INTENSIFICATION AND INDUSTRIAL BIOTECHNOLOGY

Bioprocess intensification aims to improve industrial productivity while reducing operational costs, energy consumption, and environmental impact. Advanced reactor design, integrated processing technologies, and computational optimization strategies are increasingly employed to enhance the efficiency and sustainability of industrial biotechnology processes.

Upstream and Downstream Processing

Upstream processing involves microbial cultivation, fermentation optimization, enzyme expression, and biocatalyst production. Parameters such as nutrient composition, pH, oxygen transfer, and temperature significantly influence productivity and process performance. Downstream processing includes product recovery, purification, separation, and formulation following biocatalytic reactions. Computational optimization methods assist in improving process efficiency, reducing material losses, and enhancing economic feasibility throughout industrial production systems.

In-Situ Product Recovery

In-situ product recovery techniques minimize product inhibition, improve catalyst stability, and increase overall process productivity. These methods continuously remove products from the reaction environment during biocatalytic transformations, thereby improving reaction yields and operational efficiency. Hybrid technologies integrating membrane separation, adsorption systems, solvent extraction, and biocatalysis are increasingly applied in industrial biotechnology and pharmaceutical manufacturing.

Hybrid and Multifunctional Technologies

Hybrid catalytic systems integrating chemical catalysis and biocatalysis provide promising opportunities for sustainable manufacturing and advanced chemical synthesis. These systems combine the high selectivity of enzymatic catalysis with the robustness and operational stability of inorganic catalysts. Multifunctional catalytic platforms are particularly valuable for sequential cascade reactions, pharmaceutical synthesis, biomass conversion, and environmental remediation applications. The integration of nanotechnology, computational chemistry, and enzyme engineering further enhances the efficiency of hybrid catalytic technologies.

FUTURE PERSPECTIVES

Future research in computational catalysis will increasingly rely on artificial intelligence, machine learning, high-throughput screening, and multiscale computational modeling. Integration of machine learning with quantum chemistry and density functional theory will accelerate catalyst discovery, reaction prediction, and optimization of catalytic materials. Advanced computational tools are expected to improve understanding of complex catalytic networks and support rapid screening of catalyst libraries for industrial applications.

Biocatalytic systems will continue to evolve toward multifunctional, hybrid, and highly integrated technologies capable of addressing environmental and industrial challenges. Advanced nanomaterials, synthetic biology, enzyme engineering, and computational optimization will play essential roles in developing sustainable industrial processes with improved energy efficiency and reduced environmental impact. Continuous-flow bioreactors, nanobiocatalysts, and integrated catalytic platforms are expected to transform chemical manufacturing and biotechnology industries.

The convergence of computational chemistry and biocatalysis is anticipated to create transformative solutions for renewable energy conversion, pharmaceutical synthesis, carbon dioxide utilization, environmental remediation, and sustainable chemical manufacturing. Future advancements in catalyst engineering and bioprocess optimization will significantly contribute to global sustainability goals and green industrial development.

CONCLUSION

Computational catalysis and biocatalytic transformation represent rapidly advancing scientific fields with substantial industrial and environmental significance. Density functional theory, molecular modeling, quantum chemistry, and machine learning provide detailed mechanistic understanding of catalytic reactions involving nickel, iron, and bimetallic catalytic systems. Computational investigations of methanation processes, cross-coupling reactions, transition-state energetics, and metal–organic frameworks have enabled rational catalyst design and accelerated development of sustainable catalytic technologies.

Simultaneously, nanobiocatalysts, enzyme immobilization technologies, multi-enzymatic systems, and hybrid catalytic platforms offer environmentally friendly alternatives for chemical synthesis and industrial biotechnology. Advances in nanotechnology, enzyme engineering, and process intensification have significantly improved catalytic stability, selectivity, and industrial applicability of biocatalytic systems. The integration of computational chemistry with biocatalysis is expected to continue driving innovation in sustainable catalysis, renewable energy technologies, pharmaceutical manufacturing, and environmental protection. Overall, the convergence of these disciplines represents a promising pathway toward efficient, cost-effective, and environmentally responsible chemical manufacturing for future industrial applications.

REFERENCES

1. Nørskov JK, Bligaard T, Rossmeisl J, Christensen CH. Towards the computational design of solid catalysts. Nat Chem. 2009;1(1):37-46. doi:10.1038/nchem.121.
2. Hammer B, Nørskov JK. Theoretical surface science and catalysis: calculations and concepts. Adv Catal. 2000;45:71-129.
3. Hartwig JF. Organotransition Metal Chemistry: From Bonding to Catalysis. Sausalito (CA): University Science Books; 2010.
4. Kozuch S, Shaik S. A combined kinetic-quantum mechanical model for assessment of catalytic cycles. Acc Chem Res. 2011;44(2):101-110. doi:10.1021/ar1000956.
5. Freund HJ, Meijer G, Scheffler M, Schlögl R, Wolf M. CO oxidation as a prototypical reaction for heterogeneous processes. Angew Chem Int Ed. 2011;50(43):10064-10094. doi:10.1002/anie.201101378.
6. Sheldon RA, Woodley JM. Role of biocatalysis in sustainable chemistry. Chem Rev. 2018;118(2):801-838. doi:10.1021/acs.chemrev.7b00203.

7. Bornscheuer UT, Huisman GW, Kazlauskas RJ, Lutz S, Moore JC, Robins K. Engineering the third wave of biocatalysis. Nature. 2012;485(7397):185-194. doi:10.1038/nature11117.
8. Bell AT. The impact of nanoscience on heterogeneous catalysis. Science. 2003;299(5613):1688-1691. doi:10.1126/science.1083671.
9. Corma A. From microporous to mesoporous molecular sieve materials and their use in catalysis. Chem Rev. 1997;97(6):2373-2420. doi:10.1021/cr960406n.
10. Linic S, Aslam U, Boerigter C, Morabito M. Photochemical transformations on plasmonic metal nanoparticles. Nat Mater. 2015;14(6):567-576. doi:10.1038/nmat4281.

