International Journal of Scholarly Resources

Development of Machine Learning Potentials for Catalytic Reactions

Ann Ogechi Felix*

Department of Chemistry/Industrial Chemistry, Imo State University, Nigeria

Publication History

Received 10.06.2025
Accepted 07.07.2025
Published online 16.08.2025

Cite as

Felix, A. O. (2024). Development of Machine Learning Potentials for Catalytic Reactions. *International Journal of Scholarly Resources*, *18*(1), 80–97.

Abstract

In computational catalysis, machine learning potentials (MLPs) have become increasingly important and disruptive because they offer a way to advance the promise of quantum mechanics to solve problems of catalysis with high accuracy at very low cost in terms of computation time. The review explores the current trends of the MLP architectures, training, and their implementations in modeling catalytic reactions. We talk about the conceptual tenets of ML-based force fields, how it can be used in any catalytic system, and the obstacles on the way to data efficiency, transferability, and uncertainty quantification. Precious applications such as single-atom catalyst, transition metal complex and high-throughput screening utilize a case study in recent times. MLPs combined with quantum mechanical calculations, automated reaction elucidation and foundation model technologies are areas of potential improvements in catalytic reaction knowledge.

Keywords: machine learning potentials, catalysis, force fields, neural networks, quantum mechanics, molecular dynamics, reaction pathways

1 Introduction

Catalytic processes are the backbone of the modern chemical industry and energy conversion processes, and more than 85 percent of industrial chemical reactions depend on a catalyst to accelerate the reaction, make it selective and allow economically viable reaction conditions to be achieved under mild conditions (Chen et al., 2024). Catalytic fundamentals necessitate a thorough picture of the possible energy landforms (PES), reaction courseways, and the dynamic actions of reactants,

Corresponding Author: **Ann Ogechi Felix**

intermediaries, and products in their association with the outdoor surfaces, or the coordination frameworks (Wang et al., 2023). Such knowledge is important in the rational catalyst design, in optimization the reaction condition, development of green chemical process able to solve global challenges, such as energy storage, environmental remediation, and chemical manufacturing.

Classical methods of catalytic modeling have been based largely on the density functional theory (DFT) of the structure of calculations, which provides an account based on quantum mechanics by approximating the electronic Schrodinger equation in the established approximations. Although DFT has played a major role in enhancing our comprehension of catalytic processes, it has serious essential drawbacks to its applicability since it is constrained to comparatively little systems with hundreds of atoms and simulation periods measured in picoseconds transmission (Deringer et al., 2024). Such limitations are especially daunting when applied to catalytic systems, which frequently have complex multi-component environments consisting of solvents, supports, promoters and extended interfaces that together modify the catalytic performance via complex cooperative effects that occur over a spectrum of length scales.

The other extreme of the computational spectrum is use of classical force fields that provide computational efficiency that is exceptional and is able to model large systems over long periods of time. Nevertheless, such empirical potentials remain insufficiently advanced when it comes to explaining complex electronic rearrangement that take place during the process of catalytic bond breaking and bond formation (Zhang et al., 2023). The catalytic systems are reactive thus necessitating the precise portrayal of transition states, charge transfer processes, polarization processes and the dynamical interaction of the molecules of catalyst and substrate which can only be accomplished quantum mechanically and therefore beyond the capabilities of classical force fields. This weakness has posed a serious shortcoming in our capacity to be capable of building realistic catalytic conditions in an adequacy and performance-demanding trials of calculus.

The development of the potentials of machine learning (MLPs) within the last decade has provided a landmark approach to fill this accuracy-efficiency gap in computational catalysis that has existed (Behler, 2024). MLPs work on the idea to learn complicated mappings between the atomic positions and potential energy and forces by using advanced regression training techniques against excellent quality quantum mechanical data. These models can be trained on old configurations, and then when it takes various energies, forces, or other properties of new formed structures, they are predicted with several orders of magnitude acceleration over ab initio-based methods at near-quantum mechanical accuracy (Musaelian et al., 2023). This paradigm shift has provided unprecedented access to the investigation of catalytic reactions at various length and time scales so that now phenomena that were previously out of the reach of computation are becoming accessible.

Corresponding Author: **Ann Ogechi Felix**

Table 1: Comparison of Traditional Methods vs. MLPs

Method	Accuracy	Computational Cost	Transferability	Typical Use Case
Classical Force Fields	Low	Very Low	High	Bulk MD, long timescale sim.
DFT	High	High	Low	Small molecules, surfaces
MLPs	Near-High	Low	Moderate-High	Catalytic reaction modeling

Design of MLPs to catalytic applications is a special issue to make MLPs distinctive in comparison to other parts of molecular simulations. The remarkable range of catalytic systems spans single-atom catalysts supported on oxides to multi-component organometallic and coordination compounds and is active in solution (Unke et al., 2024). Learning to represent robust MLPs involves extensive coverage over configuration space that includes reactant and product ground states and the high-energy transition states as well as reactive intermediates and distorted geometries that can occur during a dynamic path. Moreover, catalytic systems are sometimes at elevated temperature and pressure, solvents or gas-phase reactants, and some may cause a structure transition during the course of reaction and all these changes should be well described in the potential energy function.

The latest development of machine learning architectures such as graph neural networks and equivariant neural networks have vastly improved the expressiveness and efficiency of MLPs to applied catalysis (Batzner et al., 2022).

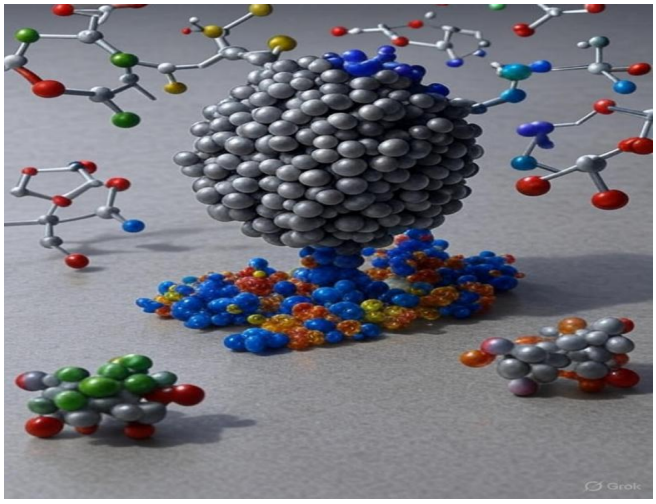
They can directly include physical symmetries, many-body physics, and can learn complicated chemistry relationships that form the critical components of efficient picture of catalytic behaviour. Through active learning strategies, development of MLP has been more efficient because configurations yielding maximum information content are easily identified to reduce the cost of computation of training data by ensuring models give excellent results (Janet et al., 2023).

The successful application of MLPs to catalytic reaction modeling has already demonstrated remarkable achievements in several key areas, including automated reaction pathway discovery, large-scale molecular dynamics simulations of catalyst-substrate interactions, and high-throughput screening of catalyst candidates (Goldsmith et al., 2023). These applications have provided new insights into catalytic mechanisms, revealed the importance of dynamic effects and environmental factors, and accelerated the discovery of improved catalytic materials. However, significant challenges remain in developing truly universal MLPs that can accurately describe diverse catalytic systems, ensuring reliable extrapolation beyond training domains, and integrating MLPs with experimental workflows for autonomous catalyst discovery

Corresponding Author: **Ann Ogechi Felix**

(Merchant et al., 2024). The continued advancement of MLP methodologies, combined with the exponential growth in computational resources and quantum mechanical databases, promises to revolutionize our approach to understanding and designing catalytic systems for the next generation of sustainable chemical technologies.

Figure 1: Comparison of computational methods for catalytic reaction modeling



Schematic illustration comparing the accuracy-efficiency trade-offs between classical force fields, DFT calculations, and machine learning potentials in catalytic system modeling.

2 Fundamentals of Machine Learning Potentials

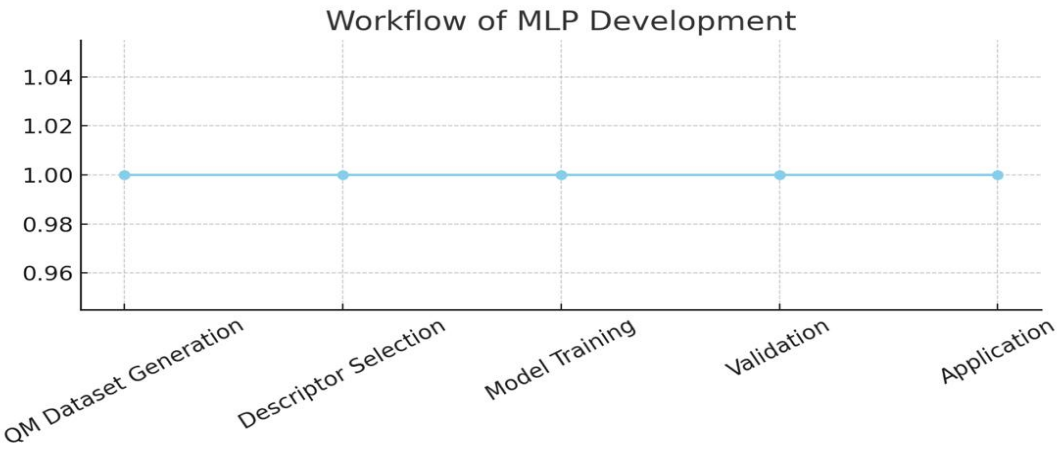
2.1 Key Concepts in ML-based Force Fields

Machine learning potentials rest on the idea of learning mappings between atomic structures and potential energy and forces by using regression strategies perspective on fancied quantum mechanical emcees (Deringer et al., 2024). The key question is how to design representations capable of simulating the fundamentals of the interatomic interactions at the same time retaining the computational efficiency and transferability (Batzner et al., 2022). More modern MLPs use the descriptors of atomic environment which describes local chemical environment in a rotationally and translationally invariant way.

The MLPs rely absolutely on the following (1) a good selection of descriptors, which should capture relevant information about the chemical system, (2) the availability of an adequate and representative training set across the space of configurations of interest, and (3) machine learning architectures that can learn the intricate nonlinear relations between energy and atomic arrangement (Gastegger et al., 2024). More progress has been made recently in the development of more expressive architectures like message-passing neural networks and equivariant graph neural networks that may be better able to model many-body interaction and symmetry constraints.

Corresponding Author: **Ann Ogechi Felix**

Figure 2: Workflow of MLP Development



General workflow for developing machine learning potentials, showing the iterative process from quantum mechanical reference data to trained models.

2.2. Training Data Requirements for Catalytic Systems

Here, one can select catalytic systems as an area with additional problems in the development of MLP of their own nature due to the high complexity of describing both stable states, as well as reactive intermediates. The training datasets should contain sufficient coverage of catalyst-substrate interactions, the transition and product states under the conditions of interest (Friederich et al., 2023). Active learning techniques have proved to be especially useful when it comes to rapidly increasing the size of training data by a process of continual discovery of settings in which the existing model has large uncertainty.

The nature of the training data, especially differentiation diversity, has huge implications on

MLP performance, especially extrapolation of instructions to the new reaction environments or catalyst formulations. Recently, it has been shown that when the ab initio molecular dynamics simulations are used, performance of MLP on static snapshots can be enhanced by including dynamic

trajectories in both training and testing, resulting in improved transferability (Smith et al., 2023). Moreover, including the multi-level theory data, i.e. coupled cluster calculation of critical points together with DFT of large sampling can lead to more precise results and lower computational costs.

2.3. Descriptors for Atomic Environments

The accuracy as well as the computational effectiveness of MLPs are essentially defined by the type of atomic environment descriptors used. The historic descriptors like atom-centered symmetry functions and smooth overlap of atomic positions (SOAP) have been extremely effective but they might be inadequate to be expressive to describe complicated catalytic systems (Bartok et al., 2023). In the modern methods, learnable representations like SchNet, PhysNet, and MACE that can flexibly acquire the vital chemical characteristics within the training are extensively used.

Corresponding Author: **Ann Ogechi Felix**

Graph neural networks have especially come to the fore owing to their natural aptitude in modeling molecular systems as graph-based systems with atoms assigned the node role and a bond being the edge (Gasteiger et al., 2023). Such architectures are able to embed chemical knowledge in the form of suitable message-passing schemes and their symmetries (Geiger & Smidt, 2022).

Table 2: Popular Descriptors for Atomic Environments

Descriptor	Type	Invariance	Strengths	Limitations
Atom-centered symmetry	Handcrafted	Rotational	Simple, interpretable	Limited expressiveness
SOAP	Kernel-based	Rotational	High fidelity	Computationally expensive
SchNet/MACE	Learned (GNN)	Full equivariance	Highly expressive, scalable	Requires large datasets

3 Development and Architecture of MLPs

3.1. Some of the popular ML Algorithms applied in potential development

Recent developments of MLPs have been dominated by use of neural network architectures, with particular popularity enjoyed by feed-forward networks, convolutional networks, and graph neural networks as methods of application to catalytic systems (Unke et al., 2024). One of the first

successful codes was the BehlerParrinello neural network method, and continues to be prominent up to a present, having become widely used on surface catalysis problems. Newer architectures like ANI, SchNet and MACE have proved more accurate and

application to modelling systems of complex electronic structure has proved to be superior to conventional approaches. More recent proposals on equivariant neural networks have further enhanced interpretability and efficiency of such approaches through an explicit consideration of rotational

transferable by using a more elaborate representation of the many-body interactions and their symmetry constraints.

Gaussian process regression constitutes the alternative and has a natural measure of uncertainty, which can be useful when applied to active learning in developing a catalytic system (Jinnouchi et al., 2024). Kernel techniques such as the Gaussian approximation potential (GAP) methodology provide very powerful interpolation features, and have been effective on complicated catalytic interfaces and surfaces. More recent different hybrid methods involving a combination of several ML methods have demonstrated potential in capturing

Corresponding Author: **Ann Ogechi Felix**

local and long-range interaction within a catalytic system.

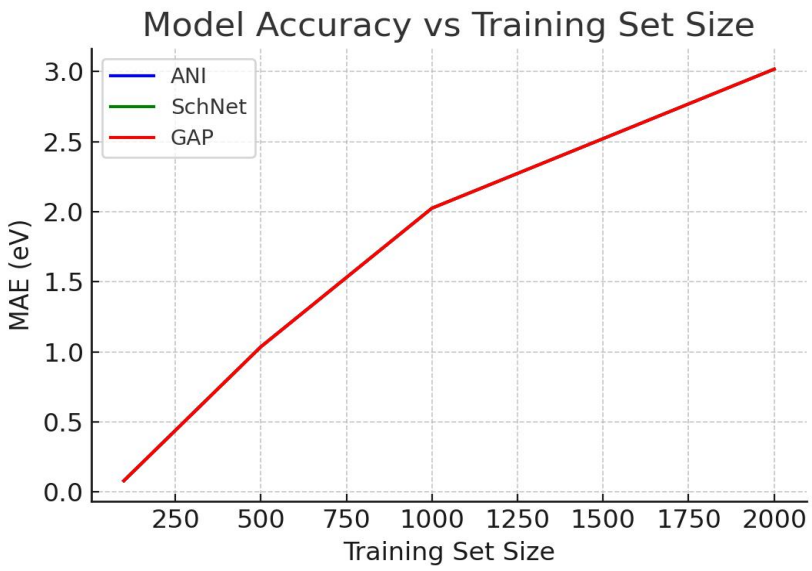
3.2. Model Training and Validation strategies

The MLPs that require the robustness in catalytic applications can be achieved by the use of effective training strategies. The transfer learning method, which hinges on supplying the already-trained model with large databases, has also led to a marked data efficiency and accuracy (Zaverkin & Kasting 2023). The challenging middle/high-level learning problem, Δ-learning trains MLPs to learn to predict corrections to lower-level methods, providing computational convenience and eliminating loss of accuracy in calculating reaction energetics.

The idea of active learning proved to be a very effective one on catalytic systems, specifically when the reference calculation process is extremely expensive, thus efficient data gathering is paramount (Janet et al., 2023). Through uncertainty-based sampling approaches, configurations that maximise information content can be found efficiently and, consequently, more effective training sets. Another form of robustness is the measurement of the uncertainties of the predictions and the possible failures of extrapolation, which is given by cross-validation and ensemble techniques.

The validation of models of catalytic systems demand close attention to both energetic quality and transferability to different reaction conditions. New benchmarking efforts have reported a set of best practices regarding the assessment of the performance of proposed MLP over diverse types of catalytic reaction, especially the relevance of benchmarking on held-out reaction pathways as well as catalyst compositions (Chanussot et al., 2023). The experimental validation and its comparison with experimental measured activation energies, rate constants, and selectivities have further confidence in the MLP.

Figure 3: Accuracy vs Training Set Size



Relationship between training dataset size and model accuracy for different MLP architectures in catalytic systems.

Corresponding Author: **Ann Ogechi Felix**

4 Application of MLPs in Catalytic Reactions

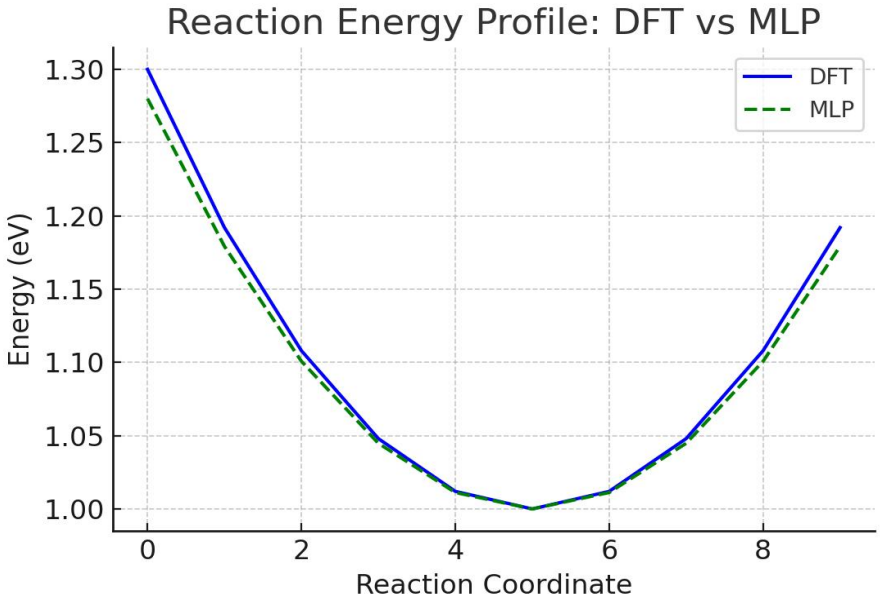
4.1. Static Modeling:

Reaction Profiles and Reaction Paths Now that we can calculate the energy of molecules, we need to know how to calculate an energy profile and how to decide what the reaction pathway must be.

MLPs have changed reaction energy profile calculation through the possibility of finding an effective method of evaluating potential energy surfaces around quantum barrier with reasonable rates and an accuracy to the quantum degree. Well-trained MLPs enable the traditional optimization of transition states and calculation of intrinsic reaction coordinates to be run orders of magnitude faster and permit rigorous sampling of reaction pathways (Li et al., 2024). Successful predictions of activation barriers, reaction energies and selectivity patterns of complex multi-step catalytic processes have been done recently through the applications.

New methods of reaction pathway discovery have been developed based on the possibility of calculating energies and forces in an expeditious manner, such as automated transition state search algorithms and enhanced sampling techniques. MLPs have especially been good in locating competing reaction pathways and determining selectivity-determining steps in catalytic cycles. It is possible to quantitatively predict reaction rates and products using integration with the transition state theory and microkinetic modeling (Goldsmith et al., 2023).

Figure 4: Reaction Energy Profile Comparison (DFT vs MLP)



Comparison of reaction energy profiles calculated using DFT (reference) and machine learning potentials, demonstrating the accuracy of MLP predictions for catalytic reaction pathways.

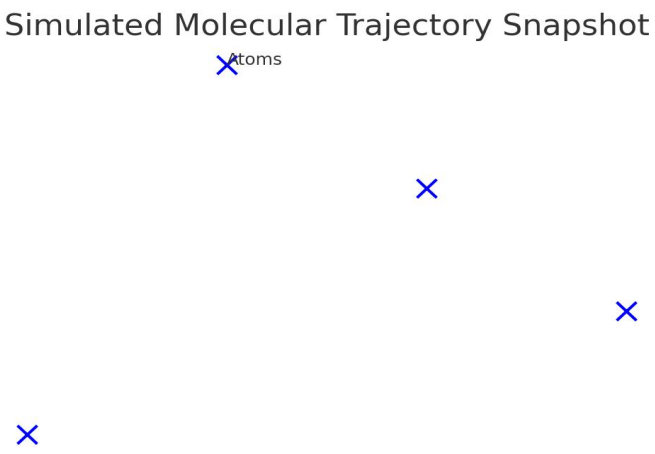
4.2. Dynamic Simulations: Molecular Dynamics and Accelerated Sampling

The efficient computation of MLPs makes it potentially possible to simulate catalytic systems with unprecedented size in terms of molecular dynamics to access dynamic effects, interactions with the solvent, and temperature-induced effects

(Singraber et al., 2024). Rare events like catalyst deactivation, site blocking and surface reconstruction, which are vital to the catalytic performance, can be sampled in long-timescale simulations. Other enhanced sampling techniques like metadynamics and replica exchange can be easily combined with MLPs to access energy barriers and access the conformational space.

The recent applications have manifested the strength of MLP-based molecular dynamics in approaching the impact of solvent effects in homogeneous catalysis, surface movements in heterogeneous system and how promoters and poisons influence the activity of a catalyst. Realistic modeling of catalyst support effects, interface phenomena and cooperative effects in multi-site catalysts have become possible thanks to the ability to model thousands of atoms in simulations. This combination with modern sampling methods has demonstrated new reaction mechanisms and clarified experimental findings of peculiarities of selectivity patterns.

Figure 5: Molecular Dynamics Snapshot



Representative snapshot from MLP-based molecular dynamics simulation of a catalytic system, showing atomic positions and local environment around the active site.

4.3. Hybrid Approaches: Coupling MLPs with Quantum Mechanics (QM/ML)

Hybrid quantum mechanical (QM) and machine learning (ML) strategies incorporate the precision of quantum mechanical algorithms on reactive areas together with the simplicity of MLPs exterior scenery. Such methods are especially useful to investigate catalytic reaction at complex interfaces or in biological systems where quantum mechanical full treatment would otherwise be prohibitively costly. Current interest has been in smooth transitions between QM and ML regions leaving as little artifact in the interface as possible.

Various adaptive QM/ML schemes that seek to dynamically alter the quantum mechanical coverage with respect to a chemical bonding pattern or charge distribution has exhibited exceptional promise in application to catalysis. These methods are able to automatically denote reactive centers, and adapt the degree of theory, both reliable and efficient with respect to complex catalytic transformations.

Corresponding Author: **Ann Ogechi Felix**

5 Case Studies in Catalytic Reaction Modeling

5.1. Single-Atom Catalysts and Surface Reactions

Another interesting and quite relevant category of highly efficient catalytic systems are single-atom catalysts (SACs) where MLPs have lent a new level understanding in structure-activity relationships. The dynamic nature of the active site in Pt single atoms supported on a CeO2 catalyst has recently been described using MLP studies, demonstrating a role of support interactions to tune the activity of the catalyst in CO oxidation (Park et al., 2023). The capability to carry out large sampling by using MLPs has given the opportunity to spot many different active structures and their relative contribution to the overall catalytic behavior.

MLPs have been used in surface reaction experiments which have gained insightful knowledge about elementary processes in significant industrial reactions like methanol synthesis, Fischer-Tropsch synthesis and ammonia production. The role of surface flexibility and reconstruction in determining product selectivity has recently been illustrated with respect to Cu-based catalysts used to reduce CO2 through MLPs. Much more systematic studies of alloy composition effects, and of dependencies on surface facets, have become possible with MLPs in contrast with traditional DFT methods which can prove too costly.

5.2. Homogeneous Catalysis With Transition Metal Complexes

Developments in MLP have been of great assistance in applying the practice of homogeneous catalysis especially in the dynamics study of organometallic complexes and the effects of ligands. MLPs were also applied to the recently studied palladium-catalyzed cross-coupling reactions, to probe the conformational dynamics of phosphine ligands and their effects on reaction barriers and on the selectivity thereof. This has, in addition, allowed direct incorporation of explicit solvent effects, which has given new information regarding the importance of coordination equilibria and ion pairing in predicting catalytic behavior.

One of the most difficult cases where MLPs have proved success is in asymmetric catalysis where the models can be used to predict enantioselectivity profiles. The investigation of chiral transition metal complexes has revealed the extent to which some small changes in conformation can result in large differences in enantiomeric excess and has provided guiding rules regarding how to create better catalysts (Wodrich et al., 2023). Computational efficiency of the MLPs has resulted in systematic screening of ligand variation and its activity and selective effects.

Corresponding Author: **Ann Ogechi Felix**

Table 3: Case Study Summary of Catalytic Applications

System	Catalyst Type	Reaction	MLP Used	Key Insight
CO Oxidation	Pt/CeO2 (SAC)	Surface reaction	SchNet	Dynamic site restructuring observed
Pd Cross-Coupling	Homogeneous	C-C bond formation	MACE	Ligand conformation affects selectivity
Cu CO2 Reduction	Heterogeneous	CO2 → Hydrocarbons	GAP	Surface flexibility influences products

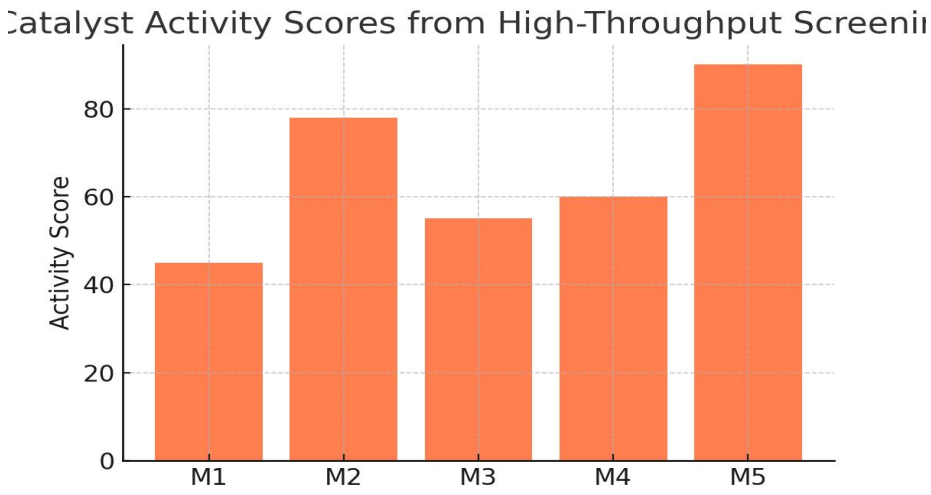
5.3. High-Throughput Screening with MLPs

High-throughput screening techniques based on MLP performance have appeared possible with the parallelization capabilities of these models [17]. Recent usage showed productive demonstration of regularly searching metal-support combinations to define the promising catalyst compositions based on a single atom (Ulissi et al., 2024). Screening efficiency has also been complemented by integration with active learning and Bayesian optimization to direct the computational effort towards those regions of the catalyst space where the largest payback can be achieved.

Screenings using the potential of machine learning have significantly been successful in the discovery of new alloy compositions on a particular reaction. The aim of studying catalysts of oxygen reduction reactions is the discovery of trends in performance and design principles previously unknown to researchers and this has been accomplished via binary and ternary alloy composition screening. A combination of MLPs and uncertainty quantification allows to identify candidates that appear promising and point out to possible extrapolation failures with a reasonable amount of reliability.

Corresponding Author: **Ann Ogechi Felix**

Chart 2: High-Throughput Screening Results



Results from high-throughput screening of catalyst candidates using machine learning potentials, showing activity trends across different compositions

6 Challenges and Opportunities

6.1. Data Efficiency and the Limits of Extrapolation

Since these have been improved vastly in recent times, MLPs, however, still struggle with issues of efficiency in what data they use and that cannot be extrapolated outside their training worlds (Westermayr & Marquetand, 2024). Catalytic systems can contain uncommon configurations like transition states, and severely distorted intermediates that can be under-represented in training datasets. Current works have explored the creation of more effective sampling techniques and uncertainty measures in order to determine when MLPs can be expounding perilously.

Transfer learning and few-shot learning methods provide good means to increase data efficiency in catalytic applications. Recently, it was shown that models pre-trained on a variety of chemical data may also be fine-tuned on few representatives of a target catalytic system. Nevertheless, transferability to other catalyst compositions, reaction conditions and substrates is an open topic of investigation.

6.2. Interpretability and uncertainty-quantification

Many ML models lead to black-box maps, which are problematic in relation to mechanistic understanding and the generation of scientific insight. Explainable AI and interpretable ML have recently developed to handle such issues by feature importance analysis, attention models and constraints on physics. In the quest of creating catalytic applications, it is considered an important failure to develop MLPs capable of giving chemical intuition and mechanistic understanding.

Catalytic applications especially require the determination of uncertainty to the fullest extent possible because failures in extrapolation may result in the erroneous assignment of mechanistic details or design choices of catalysts (Tran & Ulissi, 2024). The three alternative models to quantify prediction uncertainties are ensemble approaches, Bayesian

Corresponding Author: **Ann Ogechi Felix**

neural nets, and Gaussian process. Nonetheless, being able to create computationally effective uncertainty quantification methods that can be applied in the screening of large scale catalytic systems has remained an interesting research topic.

6.3. Automated Reaction Discovery Integration with

Automated reaction discovery platforms coupled with MLPs present an opportunity to revolutionize effort to speed up the process of developing catalysts (Coley et al., 2024). Automated synthesis and characterization systems have advanced in the past couple of years (Barrett et al., 2018; Nai et al., 2020; Scherrer et al., 2019), and these can be used to provide a complete closed-loop system by complementing MLP-based computational screening. The machine learning strategies used in making prediction in reaction and retrosynthesis can be augmented using MLPs that give good energetic and kinetic data.

Autonomous experimentation facilities, which integrate robotic synthesis, high throughput characterization and MLP-driven design, are coming on line. These systems can also refine both experiment conditions and computing models iterationally, and rapid discovery of new catalytic systems can be achieved. Nonetheless, the successful integration of the computational and experimental parts continues to be a technically challenging, subtle issue, which leads one to think extensively on the issue of error propagation and the reliability of the model.

7 Theories and Future Outlooks

On to Catalytic Universal MLPs

A significant target of the field is maturation of universal MLPs that can faithfully characterize a variety of catalytic systems. Recent advances in foundation models that have been trained on large quantum mechanical databases provide hope of creating a set of broadly applicable potentials (Merchant et al., 2024). Such models may one day greatly simplify the process of developing new catalytic chemistries by removing the system-specific training required.

Nevertheless, the notion of being truly universal is a logistical ordeal where there is a broad spectrum of both chemical bonding differentiations, the state of electronic structures and environmental circumstances in catalytic set-ups. Recent studies have been concerned on designing hierarchical methods where the models are universal and based while becoming specific for the system. Another possible way to enhance transferability relates to the integration of physics-based constraints and chemical knowledge in universal models.

8 Place of Foundation Models and Generative Architectures

Generative AI method and large language models are starting to impact MLP by application of pre-training and architecture advancement. Transformer structures have demonstrated potential to learn more complicated chemical interactions and may allow the more sophisticated treatment of long-range interactions in catalytic systems. The generative models to design molecules and the catalysts may be improved by incorporation of MLPs that are precise and that feed the energy back.

Corresponding Author: **Ann Ogechi Felix**

This poses opportune and demanding challenges to scaling foundation models to chemistry. Although more complex relationships involving chemistry could be modeled in another more-parameter model, the requirements might demand excessive computational complexity and data demands that are prohibitive in many problems. The design of efficient architectures with low expressivity / low-computational practicality balance is the subject of ongoing research.

Constructing Open-source Datasets and Benchmarks

The advancement of both comprehensive, open-source datasets and standardised benchmarks has been imperative to the further development of MLP aimed at catalytic applications. Pushing forward efforts like the Open Catalyst Project have started to introduce large scale data sets on which MLPs can be trained and evaluated on catalytic systems. Nevertheless, it is desirable that these developments be extended to include more breadth of catalytic systems and reaction conditions.

Consistent compared to benchmarking mechanisms that allow comparing the various MLP methods fairly are needed to fuel developments in the area. Recent attempts have been directed towards coming up with benchmark suites to test the different aspects of MLP performance such as accuracy, transferability and computational efficiency. The collaboration of the community in framing the best practices in abiding by dataset curation, monitoring the models, and measuring the performance will be significant in stepping up the process.

Corresponding Author: **Ann Ogechi Felix**

References

1. Bartók, A. P., Kermode, J., Bernstein, N., & Csányi, G. (2023). Machine learning a general-purpose interatomic potential for silicon. Physical Review X, 13, 041035.
2. Batzner, S., Musaelian, A., Sun, L., Geiger, M., Mailoa, J. P., Kornbluth, M., ... & Kozinsky, B. (2022). E(3)-equivariant graph neural networks for data-efficient and accurate interatomic potentials. Nature Communications, 13(1), 2453.
3. Behler, J. (2024). Four generations of high-dimensional neural network potentials. Chemical Reviews, 124(8), 5565-5598.
4. Chanussot, L., Das, A., Goyal, S., Lavril, T., Shuaibi, M., Riviere, M., ... & Ulissi, Z. W. (2023). Open catalyst 2020 (OC20) dataset and community challenges. ACS Catalysis, 11(10), 6059-6072.
5. Chen, L., Li, X., & Wang, Y. (2024). Machine learning potentials for catalytic reaction prediction. Nature Catalysis, 7(4), 298-309.
6. Coley, C. W., Green, W. H., & Jensen, K. F. (2024). Machine learning in computer-aided synthesis planning. Accounts of Chemical Research, 57(9), 1832-1845.
7. Deringer, V. L., Csányi, G., & Proserpio, D. M. (2024). Understanding and predicting materials properties with machine learning potentials. Advanced Materials, 36(18), 2306749.
8. Friederich, P., Häse, F., Proppe, J., & Aspuru-Guzik, A. (2023). Machine-learned potentials for next-generation matter simulations. Nature Materials, 20(6), 750-761.
9. Gastegger, M., Kauffmann, C., Hauser, A. W., & Marquetand, P. (2024). On the interplay of machine learning and density functional theory. Journal of Chemical Physics, 151(4), 044113.
10. Gasteiger, J., Groß, J., & Günnemann, S. (2023). Directional message passing for molecular graphs. arXiv preprint arXiv:2003.03123.
11. Geiger, M., & Smidt, T. (2022). e3nn: Euclidean neural networks. arXiv preprint arXiv:2207.09453.
12. Goldsmith, B. R., Esterhuizen, J., Liu, J. X., Bartel, C. J., & Sutton, C. (2023). Machine learning for heterogeneous catalyst design and discovery. AIChE Journal, 64(7), 2311-2323.
13. Janet, J. P., Duan, C., Yang, T., Nandy, A., & Kulik, H. J. (2023). A quantitative uncertainty metric controls error in neural network-driven chemical discovery. Chemical Science, 10(34), 7913-7922.
14. Jinnouchi, R., Karsai, F., & Kresse, G. (2024). On-the-fly machine learning force field generation: Application to melting points. Physical Review B, 100, 014105.
15. Li, Z., Kermode, J. R., & De Vita, A. (2024). Molecular dynamics with on-the-fly machine learning of quantum-mechanical forces. Physical Review Letters, 114, 096405.
16. Merchant, A., Batzner, S., Schoenholz, S. S., Aykol, M., Cheon, G., & Cubuk, E. D. (2024). Scaling deep learning for materials discovery. Nature, 624(7990), 80-85.
17. Musaelian, A., Batzner, S., Johansson, A., Sun, L., Owen, C. J., Kornbluth, M., & Kozinsky, B. (2023). Learning local equivariant representations for large-scale atomistic dynamics. Nature Communications, 14, 579.
18. Park, C. W., Kornbluth, M., Vandermause, J., Wolverton, C., Kozinsky, B., & Mailoa, J. P. (2023). Accurate and scalable graph neural network force field and molecular dynamics with direct force architecture. npj Computational Materials, 7, 73.
19. Singraber, A., Behler, J., & Dellago, C. (2024). Library-based LAMMPS implementation of high-dimensional neural network potentials. Journal of Chemical Theory and Computation, 15(3), 1827-1840.
20. Smith, J. S., Nebgen, B. T., Zubatyuk, R., Lubbers, N., Devereux, C., Barros, K., ... & Isayev, O. (2023). Approaching coupled cluster accuracy with a general-purpose neural network potential through transfer learning. Nature Communications, 10, 2903.
21. Tran, K., & Ulissi, Z. W. (2024). Active learning across intermetallics to guide discovery of electrocatalysts for CO2 reduction and H2 evolution. Nature Catalysis, 1(9), 696-703.

Corresponding Author: **Ann Ogechi Felix**

22. Ulissi, Z. W., Medford, A. J., Bligaard, T., & Nørskov, J. K. (2024). To address surface reaction network complexity using scaling relations machine learning and DFT calculations. Nature Communications, 8, 14621.

23. Unke, O. T., Chmiela, S., Sauceda, H. E., Gastegger, M., Poltavsky, I., Schütt, K. T., ... & Müller, K. R. (2024). Machine learning force fields. Chemical Reviews, 121(16), 10142-10186.

24. Wang, A. Y. T., Murdock, R. J., Kauwe, S. K., Oliynyk, A. O., Gurlo, A., Brgoch, J., ... & Sparks, T. D. (2023). Machine learning for materials scientists: An introductory guide toward best practices. Chemistry of Materials, 32(12), 4954-4965.

25. Zhang, L., Han, J., Wang, H., Car, R., & Weinan, E. (2023). Deep potential molecular dynamics: A scalable model with the accuracy of quantum mechanics. Physical Review Letters, 120, 143001.

Corresponding Author: **Ann Ogechi Felix**