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ML accelerated NORR catalyst screening: From ideal models to real electrochemical interfaces

Jingwen Jiang,[1] Pan Li,[1] and Wenlei Zhu[1,*]

[1]State Key Laboratory of Pollution Control and Resource Reuse, Frontiers Science Center for Critical Earth Material Cycling, School of the Environment and State Key Laboratory of Analytical Chemistry for Life Science, School of Chemistry and Chemical Engineering, Nanjing University, Nanjing 210023, China

*Correspondence: wenleizhu@nju.edu.cn

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Nitric oxide (NO) is a major pollutant from fossil-fuel combustion and vehicle exhaust. Electrochemical nitric oxide reduction (NORR) can convert NO into ammonia (NH_3) under ambient conditions, linking pollution control with chemical production. However, NORR is not controlled by adsorption energy alone. It involves several proton–electron transfer pathways through *NO, *NOH/*NHO, and *NH_xO intermediates (Figure 1). The hydrogen evolution reaction (HER) and, at some surface coverages, N–N coupling also compete for protons, electrons, and active sites. NORR activity and selectivity therefore depend on active-site structure, electrode potential, surface charge, interfacial water, electrolyte ions, and adsorbate coverage.

Density functional theory (DFT) is important for calculating adsorption energies and reaction free energies on ideal surfaces. Yet conventional DFT is expensive and usually examines only a few surfaces, coverages, and solvent structures. ML can extend this limited sampling by learning from catalyst structures, reaction conditions, DFT results, and experiments. After training, ML models can evaluate many candidate materials and interface states at lower cost. Constant-potential and explicit-solvent data can also support ML molecular dynamics and free-energy calculations. Thus, the prediction target should expand from catalyst structure alone to the combined effects of structure, potential, pH, cation type, solvent structure, coverage, and competing adsorbed species. The reliability of such models, however, still depends on the range and quality of the training data.

CATALYST-SPECTRUM POSITIONING AND NORR-SPECIFIC INTERPRETABILITY

NORR catalysts include single-atom catalysts (SACs), dual-atom catalysts (DACs), single-cluster catalysts (SCCs), single-atom alloys (SAAs), nanoparticles, metal and alloy surfaces, oxides, and reconstructed surfaces. Most direct NORR-ML studies still focus on idealized local active sites. SCCs and SAAs should therefore be treated as model systems rather than representatives of all NORR catalysts. Yang et al. combined DFT and ML for SCCs and developed a cluster-size-dependent Sabatier relationship, showing that cluster size changes NO adsorption and hydrogenation.[1] Liu et al. combined regression, compressed sensing, and grand-canonical DFT information to screen Ag-based SAAs, identifying Cu/Ag and Zn/Ag as promising candidates.[2]

Some design goals may transfer across catalyst families, including suitable NO activation, possible hydrogenation, HER suppression, and active-site stability. Numerical descriptors and optimal values are less transferable. SACs depend strongly on metal–support coordination; DACs may allow

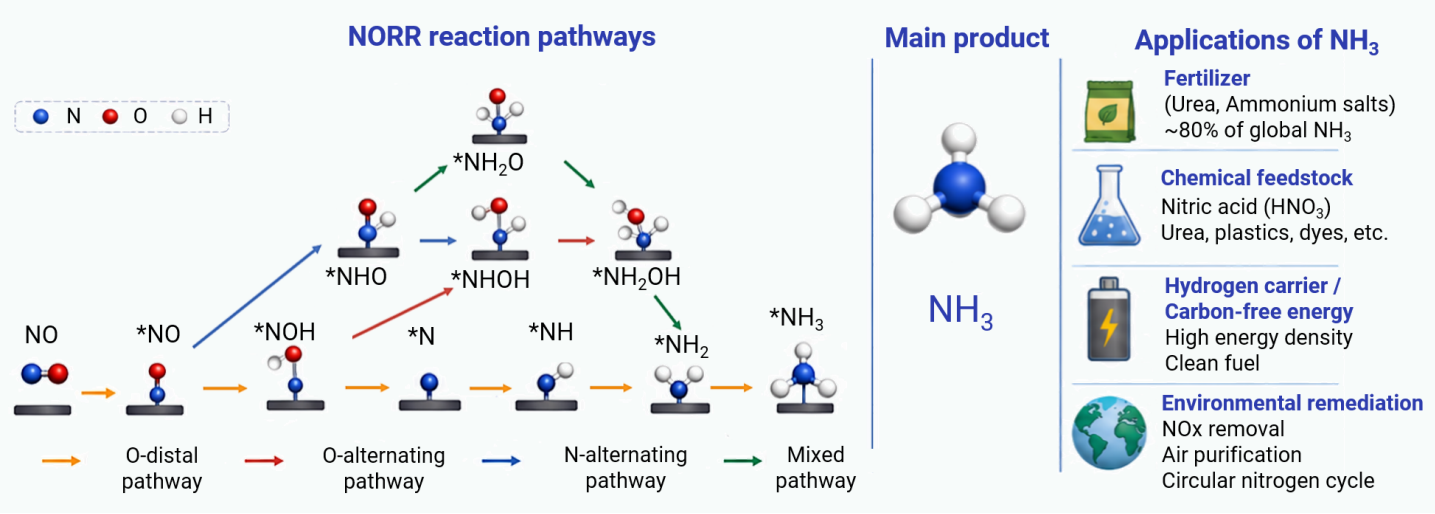

Figure 1. Reaction mechanisms of electrocatalytic nitric oxide reduction (NORR) .

bridged adsorption and cooperation between two atoms; SCCs show cluster-size and multi-atom effects; and SAAs combine ligand and ensemble effects. Surface reconstruction under operating potentials may further change the active site. Models trained on one family should therefore be tested on another family before being called general.

Model interpretation is also difficult. Most models explain theoretical targets such as adsorption energies or limiting potentials, whereas experiments measure current density, Faradaic efficiency, product selectivity, and stability. Small datasets often contain strongly related descriptors, making SHAP values or feature rankings unstable. In addition, the main pathway may change with catalyst type, potential, coverage, water, and cations. A compact SISSO equation may therefore fit the data without revealing the true cause. Reliable interpretation should combine physical rules, uncertainty analysis, tests across catalyst families, and calculations or experiments that change one factor at a time. Useful models should make testable predictions for *NO/*NOH energetics, pathway choice, HER competition, and product distribution.

NORR-SPECIFIC CHALLENGES AT REAL ELECTROCHEMICAL INTERFACES

Data shortage, simplified interface models, and weak experimental validation are common in electrocatalysis, but three features make them especially important for NORR.

First, NO is a polar radical, and *NO, *NOH/*NHO, and *NH_xO differ in

charge transfer and hydrogen-bond structure. Electric fields, cations, and interfacial water can therefore change the preferred pathway and the competition among NH_3, NH_2OH, N_2O, N_2, and HER.

Second, NORR is strongly linked to gas transport. Low NO concentration and limited transport through aqueous electrolytes make local NO concentration, gas–liquid–solid contact, wetting, and surface coverage part of the observed activity. A catalyst that performs well on a flat model surface may perform poorly in a porous electrode because of poor NO supply or flooding.

Third, practical gas feeds link selectivity with stability. O_2, SO_2, H_2O, and changes in NO concentration can block sites, cause side reactions, poison the catalyst, or change its structure. NORR models therefore need to consider reaction, transport, and deactivation together.

Recent methods show how electrochemical conditions can be included more directly. Chen et al. developed atomistic learning in the electronic grand-canonical ensemble, where system charge and grand potential depend on atomic structure and electrode potential.[3] Tian et al. combined grand-canonical DFT, explicit-solvent ML molecular dynamics, and enhanced sampling at the Ag(111)/water interface, showing that potential changes interfacial water and hydrogen bonding and thereby affects reaction kinetics.[4]

These methods still have limits. Adding potential or electron number as an input does not ensure correct charge movement, capacitance, or long-range electrostatic effects. ML also copies errors from the training data. Explicit-solvent simulations may still miss rare proton-coupled electron-transfer steps, reconstruction, aggregation, and poisoning. Their transfer to the radical and multistep NORR network remains to be tested.

FUTURE DIRECTIONS

A realistic NORR model needs data on catalyst structure, potential, charge, coverage, solvent, pH, cations, competing species, and feed impurities. CHE calculations provide broad screening, while constant-potential DFT, explicit-solvent simulations, and experiments provide higher-quality data with known source and uncertainty.

Potential-dependent ML models should link energies and forces with work function, charge, local electric field, differential capacitance, reaction barriers, microkinetic rates, and selectivity. ML molecular dynamics and active learning can guide the next calculation or experiment.

The main gap is experimental testing of new ML predictions. We found no NORR study that begins with a previously untested ML-selected catalyst and completes synthesis, structural analysis, and electrochemical NO-to-NH_3 testing. The SCC and Ag-SAA examples remain computational. A related case is the ML-guided design of B2 CuPd nanocubes for nitrate reduction, followed by synthesis and testing, reaching 92.5% NH_3 Faradaic efficiency at −0.5 V vs RHE.[5] Although not NORR evidence, it shows the standard future studies should meet.

A NORR loop should include ^{15}NO tests, analysis of NH_3 and nitrogen products, operando active-site identification, stability and impurity tests, and agreement between experiments and model inputs. ML can optimize catalyst, electrolyte, potential, pore structure, wetting, and transport. Its main value is to identify general and catalyst-specific rules and explain how the charged interface controls performance.

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DECLARATION OF INTERESTS

The authors declare no competing interests.