

SPECO: A Novel Multiparametric Methane Forecasting and Mitigation System Using Quantum Long Short-term Memory and Sonophotocatalytic Oxidation

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ABSTRACT

Anthropogenic methane (CH₄) emissions cause roughly 700,000 premature deaths annually; moreover, CH₄ is difficult to monitor and predict. Existing methods lack the predictive accuracy and real-time response necessary for effective mitigation, due to high predictive error (Khan et al., 2024). Further, few innovations currently exist to effectively reduce ambient CH₄. The goal of this study is to enhance CH₄ forecasting and mitigation efforts through SPECO, a multiparametric, dual-stage system using a Quantum Long Short-term Memory (QLSTM) neural network for accurate CH₄ hotspot prediction and sonophotocatalytic oxidation (SPECO) for CH₄ oxidation. The QLSTM neural networks were trained on 6 spatiotemporal datasets extracted from Google Earth Engine and the Emissions Database for Global Atmospheric Research, forecasting CH₄ concentrations with hyperparameter tuning. QLSTM showed a 17.37% reduction in Root Mean Squared Error (RMSE) compared to the classical LSTM baseline. The SPECO was optimized using ANSYS multiphysics software, undergoing three phases of testing: laminar flow testing using Computational Fluid Dynamics (CFD) simulations, chemical optimization using Molecular Dynamics Simulation (MDS), and vibroacoustics simulations. A physical oxidation chamber prototype was engineered using an ultrasonic transducer, yielding a 40% decrease in CH₄ as frequency increased. The novel introduction of ultrasonic cavitation was shown to enhance CH₄ oxidation by increasing reactivity through uniform propagation — an emerging solution for future space energy. The multiparametric SPECO resulted in syngas and H₂ products used for recurrent energy feedstock, supported by computational validation. SPECO is a promising dual-stage system to identify and reduce CH₄ emissions.

Keywords: Methane, recurrent neural network, forecasting, sonochemistry, catalysis.

I. Introduction

Methane (CH_4) is a potent emission released from both anthropogenic and natural sources, including industrial processes, landfills, and geological seeps, accounting for roughly 30% of global warming while having 80× more potency than carbon dioxide.¹ Consequently, a need emerges for such potent emissions to be removed from the atmosphere. While some focus on transitioning to alternative forms of energy, others — specifically industrial processes and landfills — lag in such developments.² Hence, it is necessary to introduce an implementable stopgap as such industries transition to using alternative fuels through reducing CH_4 atmospheric outputs. Additionally, methane continues to be present through emerging methane hotspots and wetlands.³ NASA sensing technology has been able to pinpoint methane hotspots, but no current strides have been made in forecasting methane concentrations from such hotspots with high accuracy.

Novel techniques such as carbon sequestration have been introduced, but lack conversion efficiency due to expensive adsorption methods.⁴ Leading carbon sequestration techniques include carbon adsorbants, which have a waning life efficiency as reaction kinetics quickly decline over time. Additionally, few algorithms have high predictive accuracy when forecasting CH_4 emission concentrations.

Photoelectrochemical oxidation (PECO) is a preexisting technique involving the use of light and electrical energy to drive oxidation reactions via reactive species such as hydroxyl radicals ($\bullet\text{OH}$).⁵ These radicals, generated at the anode, oxidize target compounds with high specificity. PECO's anodic materials, specifically those with porous nanoarrays, outperform other oxidative counterparts due to their larger surface area and abundant active sites, enabling faster reaction kinetics and greater selectivity. However, current PECO systems fail to introduce acoustics into the system, which means that reaction kinetics are less uniform and there are lower reaction kinetics.

Stage 1: Simulated Quantum Long Short-term Memory (QLSTM) Hybrid Model	Stage 2: Sonophotoelectrochemical Oxidation (SPECO) Optimization
<ul style="list-style-type: none"> ● Used to identify and predict U.S. CH_4 hotspots based on a decade of spatiotemporal trends. ● Hybrid model — classical and quantum computing integration. ● Multiparametric, spatiotemporal data based on four key features. 	<ul style="list-style-type: none"> ● Converts CH_4 into energy feedstock. ● Improving oxidation reactions through enhancing photoelectrochemical oxidation (PECO) — integrates acoustic excitation chamber. ● Overlapping sonochemistry and photoelectrochemistry.

Fig. 1. Basic research framework for SPECO dual-stage methane forecasting and mitigation system.
Graphic created by student researcher, Shanza Sami.

The goal of this study is to create a dual-stage CH_4 forecasting and mitigation system using Quantum Long Short-term Memory (QLSTM) neural networks and sonophotoelectrochemical oxidation (SPECO). This converts CH_4 into energy feedstock while addressing gaps in both environmental and energy. By integrating photoelectrocatalysis with

acoustic excitation, SPECO achieves higher efficiency and selectivity in methane oxidation reactions compared to state-of-the-art methods. The acoustic, light, and electrochemical interactions not only work in tandem with one another — but appear to have a synergistic interaction — significantly enhancing the kinetics and selectivity of these reactions while providing a sustainable solution for CH₄ mitigation.⁶

This project integrates acoustics, light, and electricity, each of which enhances the chemical oxidation of methane into syngas (H₂ + CO) and hydrogen gas (H₂), which are energy feedstocks. With enhanced reaction kinetics and low costs, SPECO will repurpose methane into energy feedstock so that methane can be perpetually reused, instead of being emitted into the atmosphere.

II. Quantum Long Short-term Memory Forecasting: Methodology

The first stage of the SPECO system was developed using a simulated hybrid Quantum Long Short-Term Memory (QLSTM) neural network, forecasting atmospheric methane concentrations across the United States. The computational framework integrated both classical and quantum layers, combining the memory capabilities of LSTMs — which capture long-term dependencies — with the parallelism and complexity of variational quantum circuits (VQCs).⁷ The datasets inputted into the model were extracted from the Google Earth Engine (GEE) and the Emissions Database for Global Atmospheric Research (EDGAR), which included Sentinel-5P NRTI HCHO, EMIT L2B, MethaneAIR L3 Concentration, MethaneAIR L4 Point Sources, and ERA5 Climate Reanalysis datasets, collectively providing multiparametric inputs.

Preprocessing involved merging and normalizing six datasets, yielding four primary variables studied for feature engineering: methane concentration, wind speed, temperature, and atmospheric pressure, all tagged with spatiotemporal coordinates. These features were standardized and encoded using Python-based extract-transform-load (ETL) decomposition, preparing the data for deep learning. The model architecture consisted of five classical LSTM neurons, whose hidden states were used as inputs to four Parameterized Quantum Circuits (PQCs), simulated using Qiskit and Pennylane. Each PQC was treated as a VQC, which enabled nonlinear function approximation and the capture of long-range temporal patterns in the data.

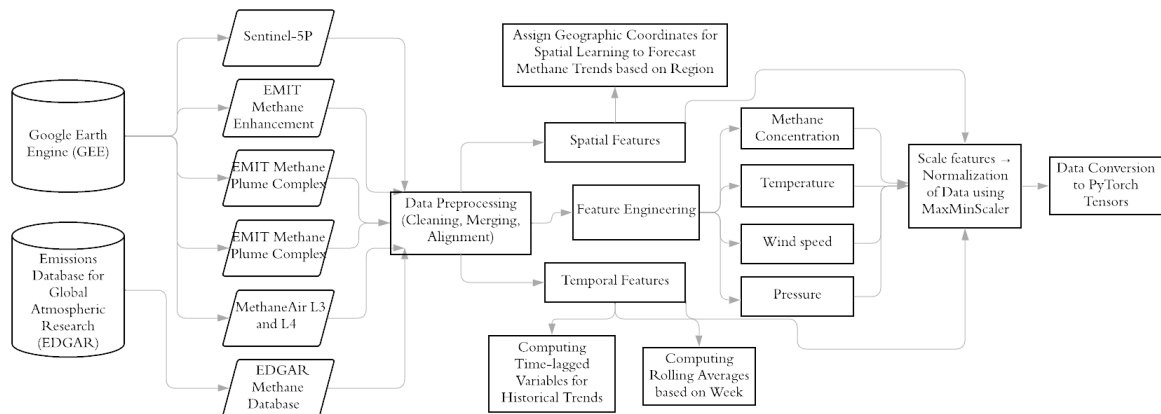


Fig. 2. The process for the initial preprocessing and state preparation. This architecture highlights the two databases the six datasets were obtained from, and key features the model was trained on.

Graphic created by student researcher, Shanza Sami.

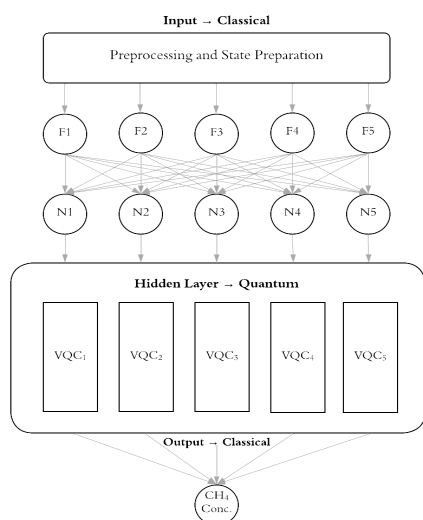


Fig. 3. The hybrid QLSTM neural network starts with classical preprocessing. The hidden quantum layer depicts variational quantum circuits (VQCs), generating one classical output in postprocessing. *Graphic created by student researcher, Shanza Sami.*

Given that the QLSTM model was simulated and hybrid, the model was able to address a common limitation in conventional LSTMs: their susceptibility to overfitting and vanishing gradients when processing complex environmental time-series data. The quantum layer processed the outputs from classical LSTM neurons, generating a postprocessed classical output signal representing the predicted methane levels. This layer was integrated with PyTorch, serving as a bridge between classical and quantum computations.

Three independent iterations of the model were tested to ensure reliability and reproducibility. These iterations were trained using an 80/20 training-to-test split, and key hyperparameters such as batch size, learning

rate, and optimizer type were optimized through manual tuning followed by the use of an Adam's Optimizer, as well as empirical validation. The model was assessed based on the Mean Absolute Error (MAE) and Root Mean Square Error (RMSE) regression model evaluation metrics compared to that of its classical LSTM baseline trained on the same inputs.

III. Sonophotocatalytic Oxidation: Methodology

The second stage of the dual-stage system focused on the development and simulation of a novel sonophotocatalytic oxidation (SPECO) chamber. SPECO uses redox reactions to reduce methane emissions by oxidizing CH_4 into hydrogen gas and syngas — both of which are common industrial energy feedstocks — using the synergistic effects observed in acoustic excitation, photocatalysis, and electrochemical charge separation. SPECO improves traditional photocatalytic oxidation (PCO) by incorporating ultrasonic excitation to enhance gas medium distribution and reaction kinetics.⁷

This four-pronged stage leverages this technology due to the high synergistic effect between the specific variables. This yielded high specificity in facilitating the desired reaction pathways, even if they were thermodynamically unfavorable. In order to model these reactions, multiphysics software was leased — specifically, COMSOL and Ansys Multiphysics software. This was designed to test each variable individually, while also observing flow distribution to determine if flow rates and prototype orientation were sound.

One of the primary factors in this methodology was ensuring uniform flow behavior and maximizing interaction between CH₄ and the catalytic surfaces. Computational Fluid Dynamics (CFD) were used to model flow behavior within the cylindrical SPECO chamber using leased Ansys software. Research parameters were iteratively refined — specifically the geometry, meshing, and inlet flow rates — to yield laminar flow propagation. Simulation parameters included Navier-Stokes equations and Reynolds number assessments to classify flow regimes, indicating laminar flow. The simulation demonstrated that

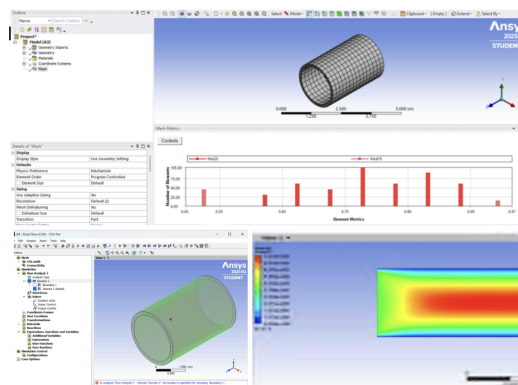


Fig. 4. CFD simulations indicated laminar flow, with acoustic notably enhancing gas propagation.
Images taken and graphic created by student researcher, Shanza Sami.

inlet-directed laminar flow, rather than flow through porous walls, was most effective in ensuring the SPECO yielded a uniform distribution of CH₄ for consistent oxidation and enhanced reaction kinetics.

To further optimize the system, previous literature and computational density functional theory (DFT) calculations by the researcher identified titanium dioxide (TiO₂) as the ideal photocatalyst. DFT results indicated that TiO₂ had the highest stability and production of reactive oxygen species (ROS); higher ROS facilitates CH₄ oxidation.

TiO₂ anatase nanopowder with 99.7% purity was obtained. The TiO₂ anatase nanopowder was incorporated into an IPA precursor, followed by a dip-coating technique onto the mesh substrate. The mesh substrate was then annealed to enhance crystallinity. This coating was inserted within the chamber where it was exposed to a UV-A LED photocatalyst, functioning by generating electron-hole pairs under UV illumination, which then produced oxidative radicals that oxidized methane into the desired syngas.



Fig. 5. TiO₂ anatase nanopowder, IPA precursor, mesh substrate.
Image taken by student researcher, Shanza Sami.

Ultrasonic transducers operating at 48 kHz were used to induce acoustic excitation within the chamber. Focused ultrasound waves created microbubbles that collapsed, leading to localized high-temperature and pressure regions, or ultrasonic hotspots. This phenomenon enhanced mass transport and surface interactions within the chamber, promoting partial oxidation of methane (POM) rather than full oxidation (FOM). The POM pathway is thermodynamically unfavorable, meaning that high temperatures and pressures will facilitate its reaction pathway. This differs from the FOM pathway, which is thermodynamically favorable, making it universally spontaneous. As a result, highly localized hotspots induced through ultrasound ultimately allowed for the POM pathway to be favorable within the reaction chamber

using relatively less energy, compared to other intensive syngas production techniques, such as steam methane reforming (SMR).

Full Oxidation of Methane (FOM)	Partial Oxidation of Methane (POM)
$\text{CH}_4 + 2\text{O}_2 \rightarrow \text{CO}_2 + 2\text{H}_2\text{O}$	$2\text{CH}_4 + \text{O}_2 \rightarrow 2\text{CO} + 2\text{H}_2$

Fig. 6. FOM and POM reaction pathways. The POM reaction pathway yields hydrogen gas and syngas, which are desired for the purpose of the experiment for continuous energy feedstock synthesis.

Graphic created by student researcher; Shanza Sami.

The chamber was engineered by the researcher, and modeled to test different configurations and frequencies. Ten 30-second trials were conducted across multiple frequencies, and CH_4 concentrations were averaged to evaluate consistency. These experiments maintained constant temperature, pressure, UV intensity, and flow rate, which isolated the SPECO acoustic effects as the tested variable. Handheld gas probes were used to analyze gas composition during testing. Results were then plotted to determine the effect of successive frequencies on the CH_4 oxidation rate.

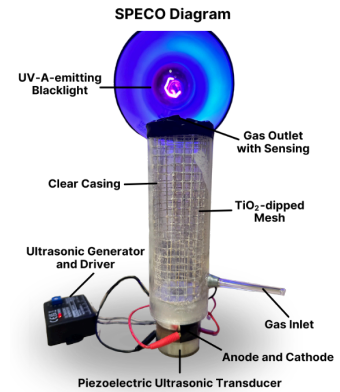


Fig. 7. SPECO chamber components.

Image taken and graphic created by student researcher; Shanza Sami.

IV. Quantum Long Short-term Memory Forecasting: Results

The performance of the QLSTM model was benchmarked against a classical LSTM baseline using key statistical error evaluation metrics: Mean Absolute Error (MAE) and Root Mean Square Error (RMSE). Across three independent iterations, the QLSTM consistently outperformed the classical baseline, demonstrating superior forecasting accuracy for atmospheric methane concentrations with an average RMSE reduction across trials of 17.37%.

When evaluation metrics were tested using a paired t-test, it identified that the QLSTM model not only generalizes better but also maintains lower variance under noisy environmental conditions. For instance, one of the trials yielded an MAE of 0.0606 and RMSE of 0.0856 for QLSTM, compared to the baseline LSTM's 0.0844 MAE and 0.1046 RMSE. This marked improvement was statistically significant, with p-values for MAE and RMSE at 0.0061 and 0.0005, respectively ($p < 0.05$).

ETL decomposition was also performed to analyze the trend and seasonality within the regression model and enhance its forecasting insight.

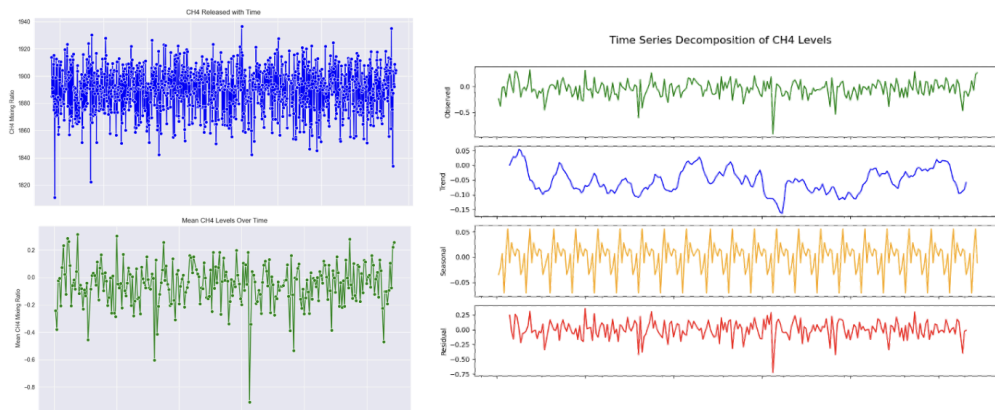


Fig. 8-10. Visualization of datasets over shorter periods of time indicates stochasticity. ETL decomposition was performed to segment data according to trends and seasonality. *Graphs created by student researcher, Shanza Sami.*

Visualization techniques and residual error analysis confirmed that the QLSTM model demonstrated tighter error margins. Moreover, performance was consistent across different data configurations, which indicates robustness to temporal and spatial variations in the test data; this is critical for models targeting environmental forecasting, where input data is often irregular.

Another important outcome was the model's responsiveness to iteration and tuning. The incorporation of quantum layers allowed the model to adapt more flexibly to complex feature interactions without overfitting. The model also converged faster during training, attributed to the expression of PQCs and their ability to model nonlinear relationships in high-dimensional data.

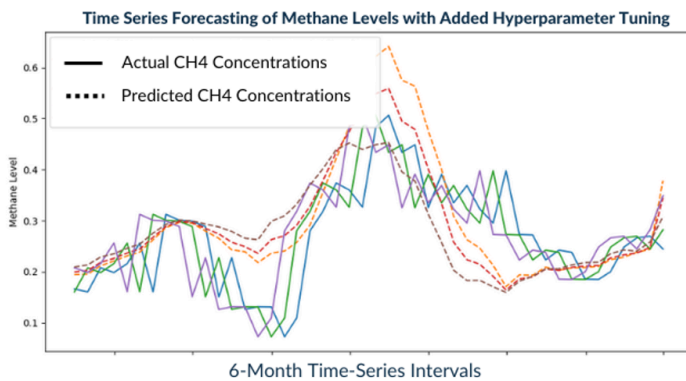


Fig. 11. Forecasting CH₄ levels across long-term time series intervals. *Graph created by student researcher, Shanza Sami.*

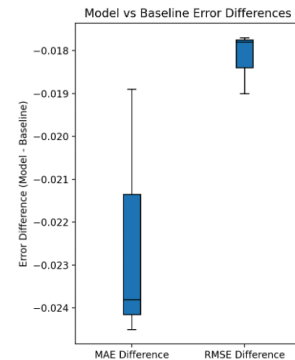


Fig. 12. Box plots modeling statistical error margins. *Graph created by student researcher, Shanza Sami.*

Furthermore, the QLSTM captured long-range dependencies across 6-month time intervals more effectively than its classical counterpart. This was evident in the time series plots generated post-inference, which closely matched observed methane values from EMIT and Sentinel-5P datasets. Heatmaps created using these forecasts also identified super-emitters accurately, aligning with known hotspot locations across the United States.

V. Sonophotocatalytic Oxidation: Results

The SPECO chamber underwent both in silico modeling and physical prototyping to validate its methane oxidation capabilities, as referenced in Section III. CFD simulations revealed that optimal performance was achieved when laminar flow was introduced through the chamber's inlet rather than its porous catalytic walls. This directional flow allowed for uniform CH₄ distribution and consistent contact with the TiO₂-coated surfaces, resulting in more efficient oxidation.

Simulation results confirmed that the flow behavior remained laminar under the selected inlet velocities, validated through Reynolds number calculations. Acoustic modeling further showed that the application of focused ultrasound at 48 kHz significantly enhanced the uniformity of medium propagation, thereby promoting effective acoustic cavitation. This uniformity is critical, as cavitation bubbles serve as microreactors where high-energy collisions drive the partial oxidation process.

Experimental results suggest that as acoustic frequency increased, the mean output of CH₄ in the chamber decreased. These results were compiled over ten 30-second trial intervals, and data were averaged to control for external variables. UV-A light intensity, chamber pressure, temperature, and gas flow rate were held constant, which isolated the observed effect of ultrasound frequency on oxidation rate. The experiments confirmed that acoustic cavitation enhanced both mass transport and catalyst-gas reaction kinetics.

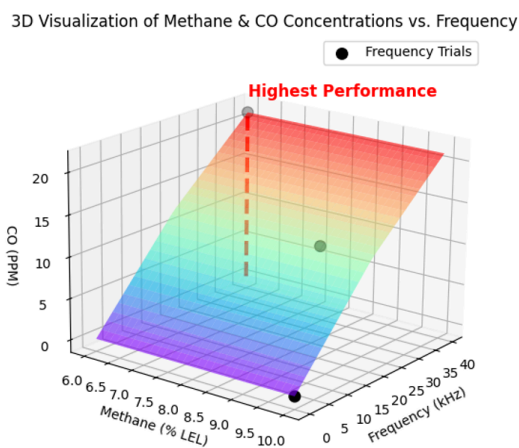


Fig. 13. Data compiled into 3D plot indicates there is a decrease in CH₄ output as frequency increases. Graph created by student researcher, Shanza Sami.

VI. Conclusions

These findings present a novel, dual-stage system that forecasts and mitigates atmospheric methane emissions by developing a simulated hybrid quantum long short-term memory model and sonophotocatalytic oxidation, with the QLSTM neural network and SPECO oxidation technique offering a predictive and mitigative solution to CH₄ emissions, respectively.

The QLSTM model demonstrated significant improvements over the classical LSTM baseline architecture, notably in terms of RMSE and MAE regression evaluation metrics. Additionally, the model can analyze complex long-term dependencies to forecast CH₄ concentrations with a lower convergence time — and notably with fewer input parameters — posing substantial implications for both scientific and industrial CH₄ tracking efforts. Future directions include obtaining more robust real-time data to ensure that the QLSTM's hyperparameters are as optimized as possible while maintaining accuracy.

The developed SPECO chamber offers a novel CH₄ conversion technique using acoustic excitation, UV-A photocatalysis, and electrochemical enhancement through TiO₂ anatase. The

SPECO selectively favors the thermodynamically unfavorable POM pathway, indicating that the SPECO presents high reaction specificity, pressure, and temperature in a synergistic effect, compared to its PECO counterpart. This makes SPECO an emerging technique to facilitate specific reaction pathways with low energy.

In conclusion, this dual-stage system could be adopted globally for real-time CH₄ management; additionally, this architecture could be modified for other pollutants or volatile organic compounds (VOCs). Future work will spearhead real-world deployment, including industrial testing of the SPECO and expansion of the QLSTM architecture for multi-class gas forecasting. SPECO could be used to generate energy feedstock in future space applications under microgravity; the acoustic excitation and high specificity of SPECO could facilitate highly specific reactions, even without rare earth catalysts.

References

- [1] The Imperative for Methane Action. (2020). Globalmethanepledge.org. <https://www.globalmethanepledge.org/imperative-methane-action>
- [2] Mahyar Kamali Saraji, & Streimikiene, D. (2023). Challenges to the low carbon energy transition: A systematic literature review and research agenda. *Energy Strategy Reviews*, 49, 101163–101163. <https://doi.org/10.1016/j.esr.2023.101163>
- [3] Zhang, Z., Poulter, B., Feldman, A. F., Ying, Q., Philippe Ciais, Peng, S., & Li, X. (2023). Recent intensification of wetland methane feedback. *Nature Climate Change*, 13(5), 430–433. <https://doi.org/10.1038/s41558-023-01629-0>
- [4] Matos, B., Batista, M., & Pires, J. (2023). Efficient adsorption of carbon dioxide and methane on activated carbon prepared from glycerol with potassium acetate. *Environmental Chemistry Letters*, 21(3), 1265–1270. <https://doi.org/10.1007/s10311-022-01556-0>
- [5] Tian, Z., Da, Y., Wang, M., Dou, X., Cui, X., Chen, J., Jiang, R., Xi, S., Cui, B., Luo, Y., Yang, H., Long, Y., Xiao, Y., & Chen, W. (2023). Selective photoelectrochemical oxidation of glucose to glucaric acid by single atom Pt decorated defective TiO₂. *Nature Communications*, 14(1). <https://doi.org/10.1038/s41467-023-35875-9>
- [6] Guan, Y., Gu, X., Deng, Q., Wang, S., Li, Z., Yan, S., & Zou, Z. (2023). Synergy Effect of the Enhanced Local Electric Field and Built-In Electric Field of CoS/Mo-Doped BiVO₄ for Photoelectrochemical Water Oxidation. *Inorganic Chemistry*, 62(41), 16919–16931. <https://doi.org/10.1021/acs.inorgchem.3c02622>
- [7] Adewuyi, Y. G. (2001). Sonochemistry: Environmental Science and Engineering Applications. *Industrial & Engineering Chemistry Research*, 40(22), 4681–4715. <https://doi.org/10.1021/ie010096l>