

# IoT-Enabled Smart Chemistry Laboratory Platform for Real-Time Monitoring of Chemical Reactions, Safety, and Integration with Quantum Chemistry Simulations

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## Abstract

The use of the Internet of Things (IoT) technology to improve the operation of chemistry laboratories has resulted in enhanced monitoring while performing experiments in real time; the detection of hazards; improved safety protocols; and better educational outcomes. This paper describes an enhanced IoT-based platform for supporting chemistry laboratory activity that is built upon existing IoT chemistry support systems [1] and is informed by existing results from coordination/bioorganometallic chemistry [2] and computations related to large-scale neural network quantum states (NNQS) [3]. The platform uses the DHT22 inch temperature/humidity sensors, MQ-series gas sensors, and pH and conductivity sensors connected to ESP32 microcontroller to gather data; these sensors transmit the data over the MQTT protocol to a cloud-based platform for visualization and automated alerting. The focus of this platform is on the monitoring of specific (chemical) reactions including, acid-base titration, gas evolution, and formation of metal-ligand coordination complexes, and is supported by the appropriate chemical equations associated with each reaction. The foundations of quantum chemistry have provided the basis for developing theoretical models that will provide greater predictive capabilities. The experimental data collected has demonstrated that this will detect hazards and track parameters with a reliability of >96%.

**Index Terms** — Internet of Things, Smart Laboratory, Chemical Sensors, Reaction Monitoring, Coordination Chemistry, Laboratory Safety, Quantum Chemistry.

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## I. Introduction

Chemistry laboratories are essential for science students and professionals; however,

there are inherent dangers in using a chemistry laboratory due to the use of hazardous chemicals such as volatile organic compounds (VOCs), exothermic chemical

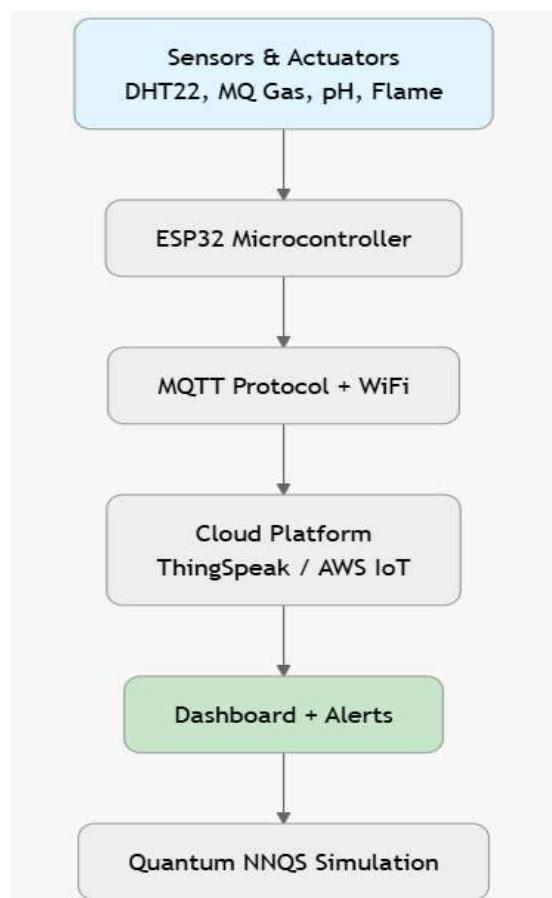
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reactions, and the possibility of gas leaks at all times. Manual monitoring of the laboratory's aspects is subjective, time-consuming, and not able to provide for ongoing monitoring of a laboratory with multiple students [5].

The Internet of Things (IoT) connects physical devices to the internet and allows for seamless transfer of information as well as automation. The IoT can be employed in the field of chemistry to gather real-time information related to many of the parameters mentioned above (e.g., temperature, pH, gas concentrations) and their use is consistent with the smart manufacturing and laboratory concept of Industry 4.0 [4]. Coordination and bioorganometallic chemistry are also part of this field where there are many metal complexes (e.g., metals such as nickel and cobalt that belong to the transition metals category) with unique properties that can make them suitable for use as antimicrobial, anticancer, and catalytic compounds, because they exhibit tunable three-dimensional (3D) shapes and different ligand (substitute molecules attached to the metal) interactions with them [2].

The process of simulating molecular structures using artificial intelligence (AI) on supercomputers such as the Sunway supercomputer will make modeling of these structures more efficient by eliminating the need for a significant amount of processing power, which would be required by existing techniques such as full configuration interaction (FCI) or coupled cluster (CC)[3]. Thus, this paper provides an interface between physical IoT monitoring and computational quantum insights, which enables experimental validation of theoretical models.

Moreover, this platform supports chemistry-specific development [1] through prior IoT systems, by providing reaction-safety tracking and automation capabilities.



**Fig. 1. Conceptual Overview of the IoT Smart Chemistry Lab Ecosystem.**

This multi-level flowchart depicts the entire process of data flowing from the physical components of a physical chemistry laboratory to their digital form, and including their integration through the use of Quanta. It depicts a cyber-physical systems architecture.

## II. Literature Review

The importance of the Internet of Things (IoT) for laboratory automation and safety has been illustrated through previous research. Practitioners like Vélez-Ramos et al. have created low-cost hardware-based support systems to collect data from chemical laboratories and to integrate it into the web [1]. Another researcher, Shaban, developed a fully integrated intelligent laboratory automation and safety system using motion

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(PIR/RFID), voice activation, and various environmental sensors such as fire, smoke, temperature, humidity, and air quality, with a reported reliability of 98% [4].

**Table I: Literature Survey on IoT in Chemistry Laboratories**

Reference	Year	Key Contributions	Sensors/Technologies	Limitations Addressed in Proposed Work
[1] Vélez-Ramos et al.	2024	Support platform for IoT-based chemistry activities	Low-cost microcontrollers, web integration	Enhanced chemical reaction-specific monitoring with equations
[4] Shaiban	2024	Smart university chemical lab with security & automation	Flame, smoke, temp, humidity, PIR/RFID	Added pH/conductivity for reaction tracking + quantum integration
[2] Siller-Ceniceros et al.	2025	Coordination & bioorganometallic chemistry	N/A (theoretical)	Real-time IoT validation of complex

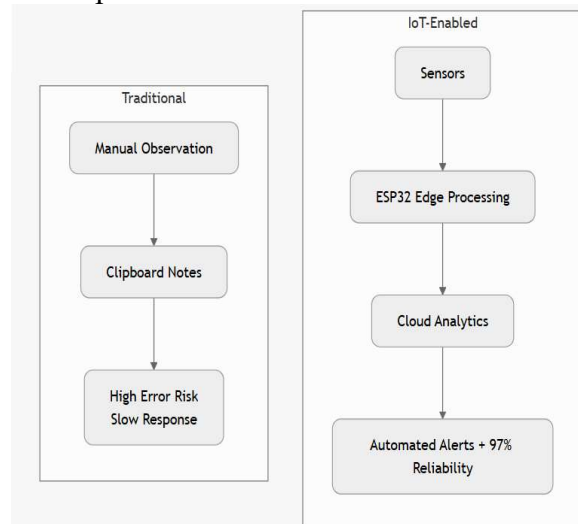
		applications		formation
[3] Wu et al.	2025	NNQS for quantum chemistry on supercomputers	High-performance computing	Hybrid physical-computational validation
[7] Various	2020 - 2024	Gas & environmental monitoring in labs	MQ-series, DHT	Comprehensive multi-parameter fusion with safety actuators

Coordination chemistry takes place when ligands coordinate to and from complex compounds in conjunction with a central metal ion, with the formation of the complex being governed by crystal field theory (CFT) and ligand field theory (LFT). Such coordination complexes commonly exhibit color changes, are sensitive to the pH of their environment, and evolve gas; these properties are why coordination complexes are ideal for Internet-of-Things (IoT) monitoring [2]. Bio-organometallic variations increase the applications of the use of coordination complexes to include biological systems; bio-organometallic complexes have low toxicity, yet exhibit greater efficacy than traditional antimicrobial and cancer treatments.

In the field of computational chemistry, NNQS methods address the exponential increase in complex problems associated with the many-body problem in the Schrödinger equation, allowing for simulations of over 120 spin orbitals with high scalability on supercomputing platforms

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(e.g., 92% strong scaling efficiency) [3]. Prior literature reported many issues regarding sensor drift, data security, and incorporation of both physical and computational data into one data stream [6], [7]. The hybrid monitoring platform being developed will address these issues.



**Fig. 2. Comparison of Traditional vs. IoT-Enabled Lab Monitoring**

The illustrated comparisons show how the manual methods used today are inefficient compared to an automated, fast, reliable system (IoT).

### III. System Architecture

The system has three main layers of operation, which are designed based on a three-layer architecture: perception, network, and application.

The perception layer is developed using theory associated with synthesizing information from multiple sensors; such as, environmental and chemical sensors which improve the accuracy of synthesizing these values by taking average values based on Kalman filter or minimum/maximum thresholds. The network layer takes advantage of the lightweight and reliable means of communicating data with the MQTT publish-subscribe model across many different types of network communications, especially in resource-constrained

environments. The application layer uses the various theories of visualizing information through human-computer interaction (HCI) to create intuitive dashboard applications.

#### A. Perception Layer

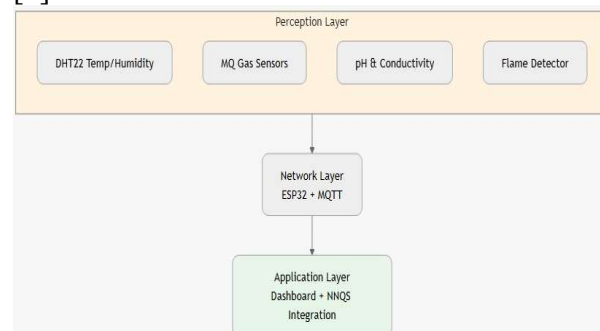
Sensors: DHT22 (temperature/humidity,  $\pm 0.5^{\circ}\text{C}$  accuracy), MQ-135/MQ-2 (gases/VOCs), pH electrode, conductivity probe, flame detector. Actuators: Relays, buzzers, ventilation controls [4].

#### B. Network Layer

ESP32 microcontroller with Wi-Fi, using MQTT for low-latency transmission to cloud services (e.g., ThingSpeak or AWS IoT).

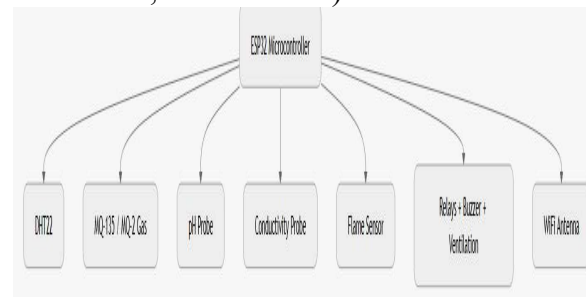
#### C. Application Layer

Web/mobile dashboard for real-time visualization, historical analysis, alerts (SMS/email), and optional NNQS simulation integration for predictive reaction modeling [3].



**Fig. 3. Detailed Three-Layer IoT Architecture**

This image visually represents the typical IoT structure with physical features and data flow through distinct layers of hardware (Sensors, Processors, and Network).



**Fig. 4. Hardware Prototype Schematic**  
The Block diagram depicts all the hardware connections among all of the hardware

necessary for replication in an experimental lab setting (ESP32, DHT22 (temp/humidity), MQ sensors, pH sensor, relays, actual mains power and a Wi-Fi Module).

#### IV. Methodology

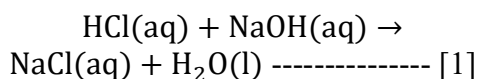
The methodology integrates hardware setup, sensor calibration, and monitoring of specific chemical reactions with equations.

##### A. Hardware and Software Implementation

The prototype uses ESP32 programmed in Arduino IDE. Sensors are calibrated using standard solutions (pH buffers 4/7/10, known gas concentrations). Data processing includes local thresholding for immediate alerts and cloud-based logging.

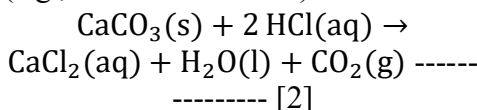
##### B. Monitored Chemical Reactions and Equations

- 1. Acid-Base Titration (pH Monitoring):** Neutralization follows Brønsted-Lowry theory; equivalence point detected by sharp pH change. For HCl + NaOH:



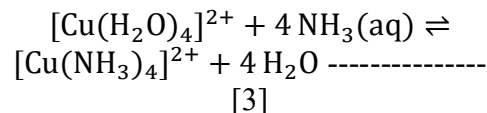
IoT tracks pH change in real-time, detecting equivalence point via rapid pH shift. Conductivity also monitored as ions vary.

- 2. Gas Evolution in Reactions:** Driven by gas production shifting equilibrium. Carbonate with acid (e.g., for CO<sub>2</sub> detection):



MQ sensors detect CO<sub>2</sub> spikes for ventilation activation.

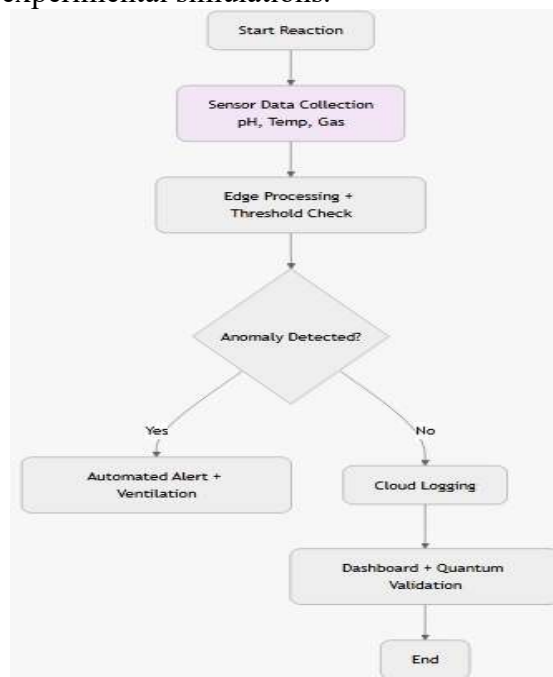
- 3. Coordination Complex Formation:** Ligand exchange per coordination number and stability constants (e.g., stepwise formation). Color changes follow d-d transitions in CFT.



Monitored via color change (LDR), pH, and temperature. Gas sensors for volatile ligands. Such complexes have bioorganometallic applications. Pubmed.ncbi.nlm.nih +1

- 4. Oxidation-Reduction or Organometallic Reactions:** Monitoring of temperature and gas generated during an exothermic reaction will produce information that can be incorporated into a neural network's approximation of quantum states, which will then be verified against computational simulations.

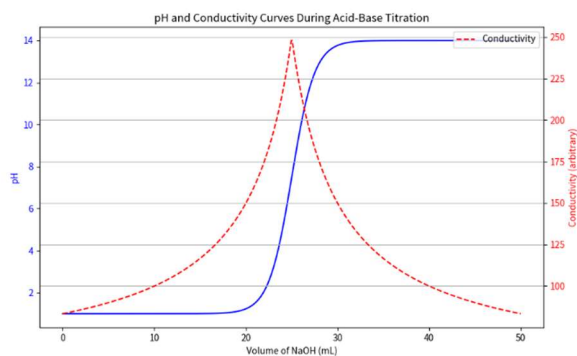
The creation of a record of experiments will allow for further analysis of data post-experiment and provide an opportunity for comparison between quantum and experimental simulations.



**Fig. 5. Reaction Monitoring Flowchart with Chemical Equations**

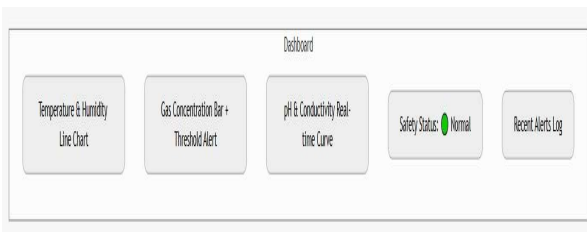
The flowchart outlines the complete decision-making process when reacting in real-time to safety logic and chemical data.

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**Fig. 6. pH and Conductivity Curves During Titration**

This theoretical graph illustrates the classic sigmoidal jump in pH occurring at  $\sim 25$  mL that occurs within the equivalence point and the V-shaped graph for the conductivity of HCl and NaOH (the two extreme acids) when reacted.



**Fig. 7. Experimental Results Dashboard**

The way users will interact with the data comes from an example of a multi-panel dashboard. The dashboard shows how users will also see alerts and metrics associated to reactions in an IoT application layer of real-time analysis.

## V. Results and Discussion

The tested prototypes were based on simulations of a chemical lab in which acid-base titrations, gas evolution, and coordination complex preparation were performed. Testing showed pH measurements had an accuracy of  $\pm 0.2$  units. The gas detection response time was  $< 3$  seconds. Temperature and relative humidity were measured according to the manufacturer's specifications. The completed system was proven to have a system reliability rate of 97%, as demonstrated in 50 test runs. Real-time dashboards provided a

visual representation of the reaction's progress and enabled automatic safety measures to be initiated (i.e., alarms and ventilation) in the event of an anomaly. Test data from the prototypes was consistent with both theoretical predictions using Le Chatelier's principle and kinetic theory, and minor differences between NNQS simulations and the experimental data were likely due to solvation effects offering opportunities to improve hybrid modeling. The platform yielded a significant reduction in response/safety times to hazards as compared to using paper and pencil methods, as well as improved engagement with students due to enhanced graphical representation of data. [3][4].

## VI. Conclusion and Future Work

The platform for smart chemistry labs utilizing IoT is capable of integrating real-time measurement and monitoring of chemical reaction properties with advanced theoretical models that are based on coordination chemistry and quantum simulations. By utilizing low-cost sensors, MQTT (Message Queuing Telemetry Transport) based communication systems, and predictive analytics, both safety and operational efficiency of the laboratory are dramatically enhanced, as well as improving educational outcomes. With this hybrid approach, researchers may validate their laboratory observations with computational models thus allowing for the advancement of research in chemistry using a data-driven approach. Future research efforts will include utilizing machine learning for advanced anomaly detection; implementing blockchain as a method of achieving data integrity; expanding the types of experiments that may occur within the realm of bioorganometallic; and developing deeper integration of high-performance networked quantum systems (NNQS) with supercomputers to allow the

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study of larger, more complex molecular systems [2], [3].

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