

AI and Quantum Research Center (AIQRC), Asia University, Taiwan

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Activity

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Time/Place: Nov. 13-14, 2025, Asia University, Taichung

Title: INTERNATIONAL SYMPOSIUM ON QUANTUM AI &amp; THE FUTURE OF LIFE

Registration is Free. Will provide the link to register in the next newsletter.

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**Awards & Achievements**

Asia University proudly congratulates **Ms. Aninda Astuti**, Ph.D. student in the **Department of Bioinformatics and Medical Engineering** and member of the **AI and Quantum Research Center (AIQRC)**, for receiving the **Best Paper Award** at the *2025 Second International Conference on Artificial Intelligence for Medicine, Health, and Care (AIxMHC)*, held on **October 13–15, 2025, in Taichung, Taiwan**.

Her paper, “*Enhancing the Performance and Speed of Quantum Support Vector Classifier via Neural Quantum Embedding and Tensor Network*,” introduces a hybrid quantum framework that integrates **Neural Quantum Embedding (NQE)** and **Tensor Network (TN)** techniques to enhance the efficiency and classification accuracy of **Quantum Support Vector Classifiers (QSVCs)**. The study highlights the potential of combining **quantum machine learning** and **tensor-based optimization** for the effective analysis of complex biomedical data.

This research was conducted in collaboration with **Professor Tai-Yue Li (National Center for High-Performance Computing (NCHC, Taiwan), , Simon See (NVIDIA) and Ka-Lok Ng (AIQRC)**.



## ***Recent progress in quantum computing***

Researchers at Tohoku University developed a multi-target quantum compilation algorithm that allows a quantum processor to optimise multiple objectives simultaneously—an important step for QML systems dealing with complex, multi-variable tasks.

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A team at Tsinghua University proposed a quantum generative model that promises exponential improvements over classical generative models for certain problems.

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On the experimental side, a photonic quantum processor from University of Vienna demonstrated a measurable performance boost in a kernel-based machine learning task, hinting that even near-term quantum devices may offer advantages in QML.

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In terms of ecosystem support, D Wave Quantum released a developer toolkit linking quantum computing with the PyTorch ML framework—simplifying how QML experiments can be deployed. (SCM Demo) The field remains exploratory rather than mature, but these developments show QML is moving from theory toward practical demonstrations.

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## **Dynamic Quantum Circuits: A Novel Approach to Molecular Generation**

The generation of chemical molecular structures is fundamental to advancements in drug design, materials science, and related fields. Although several generative models have been developed to propose new molecules, exploring the vast chemical space using classical methods requires extensive molecular datasets, significant computational resources, and a large number of model parameters, which can limit their efficiency.

Recently, a novel approach leveraging quantum computing has been introduced: the Quantum-based Molecular Generator (QMG). Drawing inspiration from Variational Quantum Circuits (VQC), QMG incorporates Y-gate rotations into a quantum dynamic circuit, allowing the learnable rotation angles to be tuned according to user-defined objective functions. By applying Bayesian Optimization (BO) to iteratively update circuit parameters based on measurement outcomes, QMG gradually converges toward optimal molecular configurations.

A key advantage of this approach is its ability to keep certain parameters fixed, thereby preserving a specific molecular scaffold. This feature is particularly valuable when optimizing target properties while maintaining a desired structural backbone. Moreover, by utilizing qubit reuse, the quantum dynamic circuit achieves both high validity and uniqueness — exceeding 90% — in generating molecular structures containing up to nine heavy atoms, including carbon, nitrogen, and oxygen.

Remarkably, this performance is achieved using only 20 qubits and 134 parameters, which is significantly fewer than the approximately 90 qubits required by static circuits. By combining quantum circuit flexibility, iterative optimization, and scaffold preservation, QMG demonstrates a highly efficient and precise approach for molecular generation, offering substantial potential to accelerate research in chemistry, drug design, and materials science.

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Prepared by Mr. Shen, Miss Aninda Astuti and Professor Ka-Lok Ng, Vice Director, AIQRC & Department of Bioinformatics and Medical Engineering, Asia University.

AI and Quantum Research Center (AIQRC)

Room A110, Asia University, No. 500, LiuFeng Rd., WuFeng Dist., Taichung City 41354 Taiwan.

Email: [qphys.qcomp@gmail.com](mailto:qphys.qcomp@gmail.com) Office: 04-23323456 ext. 6631

Web: <https://quantum.asia.edu.tw/>