

# SymQNet: VQE Hamiltonian Estimation for Molecular Optimization with Quantum Computing

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## Introduction

### Real Stakes: Drug Discovery is Broken

**\$2.6B** Average Drug Cost  
**12yr** Time to Market  
**90%** Failure Rate

A key process in drug discovery is **Molecular geometry optimization (MO)**

- Finds most stable molecular structure by **minimizing ground-state energy**

Computation models (DFT) **significantly struggle** with weak intermolecular forces.

- VQE can solve this via quantum computing, but **requires many energy estimations** for minimization.

Estimations require potentially **millions of slow measurements** to reduce statistical error.

Choosing informative measurements optimally could **mitigate the effect of this bottleneck**.

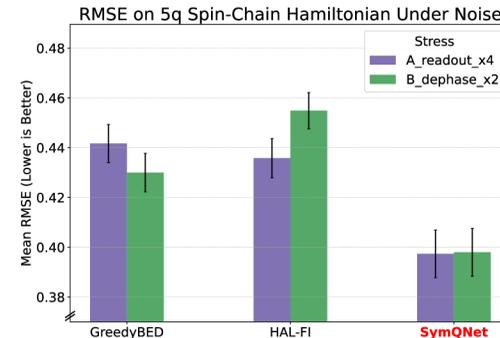


**Choose Measurement**  
Usually chosen poorly, wasting shots later  
**Pain Point**

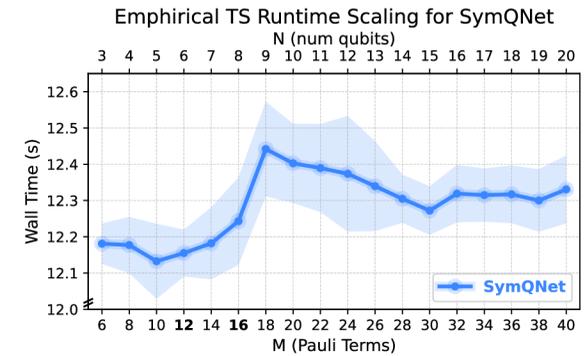
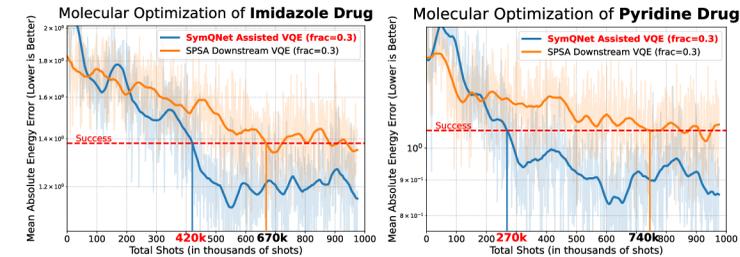
**Conduct Measurement**  
...on chosen qubit. expensive but essential.

## Key Results and Statistical Analysis

**46.7%** Shot Reduction ( $p < 0.05$ )  
**21.2%** MAE Reduction ( $p < 0.05$ )  
**1.88x** Drug Discovery Speedup



Beats baseline energy estimation methods even under **quantum noise** (statistically significant).

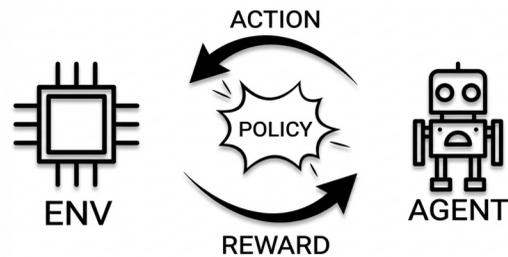


- **Cost is empirically flat** as qubits and pauli-terms grow!
- **Applicability potential to larger molecules.**

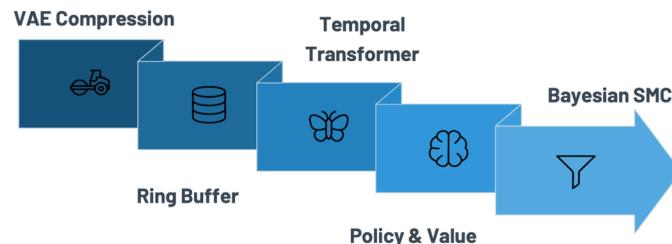
## Methodology

### Hypothesis is Based on Reinforcement Learning to Select Measurements

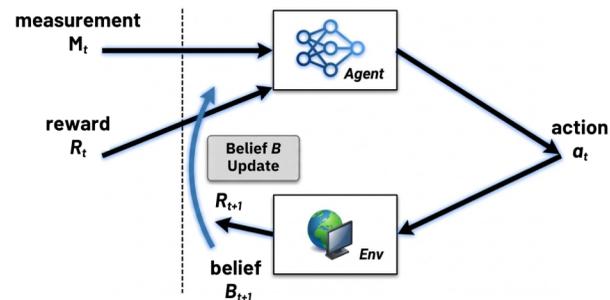
**Core Idea:** Learn a **strategy** to choose which measurements give the **most information** to estimate energy **faster**.



Reinforcement learning trains an "agent" to take **optimal actions** based on observations of its environment guided by a reward signal.



### Partially Observable MDP (POMDP) Formulation



## Hypothesis Supported, Vision Established

- Drug Discovery Speedup:** 1.88x more molecules; 46.7% VQE shot reduction
- Beats state-of-the-art:** Lower RMSE than HAL-FI, GreedyBED in quantum noise
- Empirical O(1) Scaling:** Improves from  $O(N^4)$  &  $O(M)$  baseline scaling to 20 qubits

### Reproducibility

How can SymQNet be accessible?

### Install in One Line

```
pip install symqnet-molopt
```

SymQNet is currently **patent-pending**

### My Future Vision

- Higher-Dimensional Hamiltonians**  
Train on larger, more complex molecular systems
- Real-Life Deployment**  
Trade off reward with device cost on actual quantum hardware