

科技部

111年度大專學生研究計畫申請書

一、綜合資料：

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	學 生 研 究 計 畫 名 稱	Quantum Neural Network on Electronic Structure Problem with Daubechies Wavelet Method		
	研 究 期 間	自111年7月1日至112年2月底止，計8個月		
	計 畫 歸 屬 司 別	自然司		
	研究學門代碼及名稱	M031100A1 -- 量子資訊－理論		
	上年度曾執行本部大專學生研究計畫	否		
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補助經費	項 目	金 額	說 明	
	研 究 助 學 金	48,000元	每月補助研究助學金新臺幣6,000元，8個月計新臺幣48,000元。	
	耗材、物品、圖書及 雜項費用	20,000元	依研究計畫實際需求擇優補助，每一計畫最高以補助新臺幣20,000元為限。	
	合 計	68,000元		

二、研究計畫內容

(一) 摘要

1. 摘要

隨著量子硬體 (Quantum Hardware) 的快速發展，許多量子計算化學領域 (Quantum Computational Chemistry) 的演算法得以實行。然而在量子誤差修正 (Quantum Error Correction) 方面的困難，導致現今唯有一相對完善的半量子式演算法 (Variational Quantum Eigensolver, VQE)，得以計算出給定 Hamiltonian 的最低本徵值，同時能運行於近代的量子硬體上。因此，為了讓計算資源的利用達到最佳化，使用高效基底集 (basis sets) 來分析化學分子 Hamiltonian 的過程就在電子結構問題 (Electronic Structure Problem) 中成為了重要手段。然而，當前特定的 VQE 演算法，包括以 Daubechies wavelet 基底集搭配高效率的編碼方式運行於參數化的量子電路 (Parameterized Quantum Circuits, PQCs) 之量子硬體上，或是以化學式啟發 (chemical-inspired) 所建構之 PQC 運行於模擬器上，都僅能在結構相對較小的分子上達到化學準度 (chemical accuracy)。因此，本研究引入量子神經網路 (Quantum Neural Network) 模型，同時搭配 Daubechies wavelet orbitals 之計算，來達成高效且準確的分子相關性質計算。本研究預期生成的模型準確率、所需量子位元數 (qubit number)、量子電路之深度、與量子雜訊容忍性能等層面都能與先前的研究相比擬或甚至更加突破；同時，將未監督式學習 (Unsupervised Learning) 結合 Daubechies wavelet molecular orbitals 之方法亦是前所未有的嘗試，有望為相關的問題開創新的研究方向。

2. Abstract

As the rapid evolution of quantum hardware industry, various algorithms in quantum computational chemistry are put forward for rigorous implementation. However, due to lack of quantum error correction, a promising hybrid quantum-classical algorithm to find the lowest eigenvalue of a given Hamiltonian for near-term quantum hardware is the variational quantum eigensolver (VQE). To get the best performance out of limited computational resources, using efficient basis sets to represent molecular Hamiltonian in electronic structure problems has become a crucial step. Some particular VQE calculations using Daubechies wavelet basis sets and efficient encoding schemes implemented via hardware-efficient parameterized quantum circuits (PQCs) on real quantum machines or via chemical-inspired PQCs on simulators to date are only accomplishing chemical accuracy on relatively small and simple-structure molecules. Hence, in this research we introduce a quantum neural network method while adopting the top pioneering basis sets of Daubechies wavelet orbitals for accurate and efficient quantum computations of molecular properties. It is expected that the results of this work would be comparable with or better than those of the previous works on model accuracy, required qubit number, circuit depth and quantum noise tolerance. Moreover, this work exploits the novelty of combining Daubechies wavelet molecular orbitals method with unsupervised learning on quantum neural networks, which may hold the potential to develop a new area of research

on relevant topics.

(二) 研究動機與研究問題

1. 研究動機

Due to the rapid evolution of quantum hardware industry, quantum computing has attracted much attention recently. Quantum computation of molecular properties is one of the most promising quantum computing applications. Among various methods in quantum computational chemistry, choosing a suitable and efficient basis set to represent the molecular Hamiltonian has played a key role in electronic structure problem.

One of the promising algorithms for near-term quantum hardware is the Variational Quantum Eigensolver (VQE) [1, 2, 3]. VQE is a hybrid quantum-classical algorithm as it uses the quantum computer for a state preparation and measurement subroutine, and the classical computer to process the measurement results and update the quantum computer according to an update rule. This exchanges the long coherence times needed for phase estimation for a polynomial overhead due to measurement repetitions and classical processing [3]. Currently the minimal STO-3G basis set is commonly used in benchmark studies because it requires the minimum number of spin orbitals, and thus minimum number of qubits and minimum circuit depth. Calculations using minimal basis sets are of limited accuracy, and thus can not provide useful prediction on the system properties (e.g. ground state energy, bond length and angle, molecular vibration frequency).

Some particular VQE calculations using different basis sets or encoding schemes [4, 5] implemented via hardware-efficient parameterized quantum circuits (PQCs) [3] on real quantum machines or via chemical-inspired PQCs [3] on simulators to date are only accomplishing chemical accuracy on relatively small and simple-structure molecules (e.g. H_2 , LiH). There is still room for improvement on efficiently harvesting the power of resource-saving basis functions (e.g. Daubechies wavelet orbitals) and novel variants of the VQE method.

Thus, to further enhance the overall performance in model accuracy, required qubit number, circuit depth and quantum noise tolerance, this work aims to apply hybrid quantum-classical neural networks to the quantum circuit with chosen basis sets [6]. With the help of unsupervised learning on neural networks, some characteristics that are not considered by previous chemical-inspired UCCSD-VQE based method may be included into the model, while some other redundant features could be discarded. As a result, both model accuracy and circuit complexity would outperform previous researches.

2. 研究問題

In this work, we follow the problem formulation used in [6]. The molecular “potential

energy surface” problem can be described as follows:

Input: The bond lengths of the considered molecules. The cost function to be minimized in the lowest eigenvalue problem of the VQE algorithm is defined as

$$f = \sum_j \langle \phi_j | H_j | \phi_j \rangle, \quad (1)$$

where $|\phi_j\rangle$ is the final state of the proposed hybrid quantum-classical neural networks with the j^{th} bond length as input, with H_j being the corresponding Hamiltonian.

Output: A sequence of “potential energy surface” that plots the ground state energy of the molecule with respect to a range of bond lengths.

Evaluation: The accuracy of the method is validated by comparing the results using the generated sequence of ground state energy and those performing the actual laboratory experiment, within the error bound of 1 kcal/mol regarded as chemical accuracy. In addition to the chemical accuracy, the circuit size, the runtime on real machine and qubit number used during the model generation and calculation are also crucial indicators. Note that there exists a trade-off among the indicators.

(三) 文獻回顧與探討

1. Encoding Hamiltonians

(1) The Second Quantization

Observables must be independent of the representation used. Therefore, the expectation values of second quantized operators must be equivalent to the expectation values of the corresponding first quantized operators. As first quantized operators conserve the number of electrons, the second quantized operators must contain an equal number of creation and annihilation operators. We can use these requirements to obtain the second quantized form of the electronic Hamiltonian [7, 8]:

$$H = \sum_{p,q} H_{pq} a_p^\dagger a_q + \frac{1}{2} \sum_{p,q,r,s} H_{pqrs} a_p^\dagger a_q^\dagger a_r a_s, \quad (2)$$

with

$$h_{pq} = \int d\mathbf{x} \phi_p^*(\mathbf{x}) \left(\frac{\nabla^2}{2} - \sum_I \frac{Z_I}{|\mathbf{r} - \mathbf{R}_I|} \right) \phi_q(\mathbf{x}), \quad (3)$$

$$h_{pqrs} = \int d\mathbf{x}_1 d\mathbf{x}_2 \frac{\phi_p^*(\mathbf{x}_1) \phi_q^*(\mathbf{x}_2) \phi_r(\mathbf{x}_2) \phi_s(\mathbf{x}_1)}{|\mathbf{r}_1 - \mathbf{r}_2|}. \quad (4)$$

The first integral represents the kinetic energy terms of the electrons and their Coulomb interaction with the nuclei. The second integral is due to the electron-

electron Coulomb repulsion.

(2) The Daubechies wavelet (DW) molecular orbitals

Atomic orbitals are an intuitive choice of basis set for isolated molecular systems. However, basis sets constructed from atomic orbitals suffer from non-orthogonality and hence require additional computations of the overlap matrices. Daubechies wavelets provide an alternative option for basis sets in computational quantum chemistry [9, 11, 10]. In wavelet theory, there are a scaling function $\phi(x)$ and a wavelet $\psi(x)$,

$$\phi(x) = \sqrt{2} \sum_{j=1-m}^m h_j \phi(2x - j), \quad (5)$$

$$\psi(x) = \sqrt{2} \sum_{j=1-m}^m g_j \phi(2x - j), \quad (6)$$

where the coefficients h_j and $g_j = (-1)^j h_{-j+1}$ are elements of the filter characterizing the m^{th} order of the wavelet family. There are several advantages of Daubechies wavelets: (1) the wavelets are localized in both real and reciprocal space, which is conducive for providing an accurate representation of molecular Hamiltonian in spatially localized grid points. (2) the completeness of the Daubechies wavelet basis set eliminates the superposition error induced by the incompleteness of other previously used basis sets (e.g. STO-3G). (3) the DW method has its adaptivity within programming, making chemical accuracy achievable at affordable computational cost.

2. Quantum Machine Learning (QML)

(1) Parameterized Quantum Circuits (PQCs)

A parameterized quantum circuit (PQC) is a quantum circuit consisting of data encoding gates, entangling gates and parameterized gates (i.e., gates with tunable parameters) with fixed depth. In general, an n -qubit PQC can be written as

$$U(\vec{\theta}) |\psi\rangle = \left(\prod_{i=1}^m U_i \right) |\psi\rangle, \quad (7)$$

where $U(\vec{\theta})$ is the set of universal gates, m is the number of quantum gates, $\vec{\theta}$ is the set of parameters $\{\theta_0, \theta_1, \dots, \theta_{k-1}\}$ with k being the total number of tunable parameters, and $|\psi\rangle$ is the initial quantum state. The operation of U can be modified by changing parameters $\vec{\theta}$. Thus, by optimizing the cost function with the parameters used in $U(\vec{\theta})$, PQC approximates the wanted quantum states.

(2) Constructions of the Circuit

Our PQC consists of three parts: the data encoding part, the variational circuit part, and the measurement part. One can use the hardware-efficient ansatz [3] and the variational encoding [12] technique to decrease the depth of the quantum circuit so that it can be implemented on noisy intermediate-scale quantum (NISQ) [13] devices. The classical part of the circuit is enabled by measuring the expectation values of the concerned operators. Notice that non-linearity is introduced into the circuit via direct measurement operation, which is crucial in boosting the function space of the neural network. The construction of the proposed hybrid quantum-classical neural network is illustrated in Figure 1 where the linear part in the classical neural network is replaced by the quantum circuit and the nonlinear part is replaced by the quantum measurement.

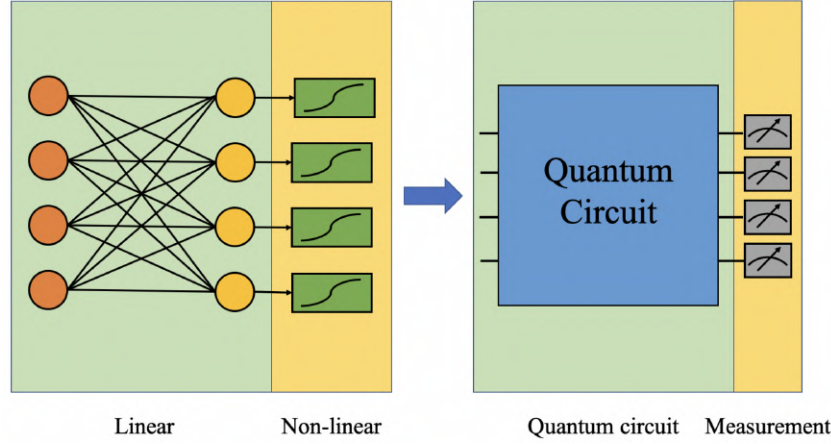


Figure 1: Quantum-classical hybrid neural network, the linear part in the classical neural network is replaced by the quantum circuit and the nonlinear part is replaced by the measurement. From [6].

(四) 研究方法及步骤

1. 研究方法

(1) Orbital Integrals

We will calculate the orbital integrals in the second quantization Hamiltonian by Daubechies wavelet (minimal) basis orbitals with [14] as reference, and with other sets of basis (e.g. STO-3G) for final result comparison.

(2) Mapping Operators

Once the calculations of orbital integrals are done, we apply second quantized basis set encoding methods, such as the Jordan-Wigner or Bravyi-Kitaev encoding method, to map from operators that act on indistinguishable fermions to

operators acting on distinguishable qubits to obtain the corresponding Hamiltonian in the Hilbert space of the qubits [3]. One may utilize the OpenFermion package [15] during the encoding procedure.

(3) Implementation of Quantum Neural Networks

To train a quantum neural network model on a hybrid circuit, we need to define a reliable network architecture. The observation is that the state space in quantum computing increases exponentially with the number of qubits, while the complexity of a classical neural network increases exponentially with the number of neuron layers in the neural network. Since increasing the number of layers of the variational part circuit (composed of entangling gates and parametrized gates) would reach saturation and may not improve the performance when the number of layers is large enough [16], we aim not to increase the depth of the circuit, but to develop a hardware-efficient hybrid network which saves computational resources while maintaining essential non-linearity. In this work, we may choose the measurement operation as means of implementing non-linearity into the circuit and use the expectation values of operators on each qubit of the PQC to serve as the nonlinear operations connecting different quantum layers. The expectation values of operators capable of extracting useful information from the PQC are used as the input data for the encoding part of the next quantum circuit layer. As for the data encoding part, we may initialize the input state as $(\otimes_{i=0}^{n-1} R_y(a)H) |0\rangle^{\otimes n}$, where a is the bond length, H is the Hadamard gate, and R_y is the rotational- y gate. The number of qubits n is equal to the number of qubits of the corresponding Hamiltonian.

For the variational part of our PQC, we may construct a circuit consisting of R_y and CNOT gates, which can be written as [6]

$$\prod_{j=0}^{n-1} \left(\otimes_{i=0}^{n-1} R_y(w_{i+n \times j}) \right) (\text{CNOT}_{n-3,n-2} \cdots \text{CNOT}_{3,4} \text{CNOT}_{1,2}) \cdot (\text{CNOT}_{n-2,n-1} \cdots \text{CNOT}_{2,3} \text{CNOT}_{0,1}) , \text{ for even } n, \quad (8)$$

and

$$\prod_{j=0}^{n-1} \left(\otimes_{i=0}^{n-1} R_y(w_{i+n \times j}) \right) (\text{CNOT}_{n-2,n-1} \cdots \text{CNOT}_{3,4} \text{CNOT}_{1,2}) \cdot (\text{CNOT}_{n-3,n-2} \cdots \text{CNOT}_{2,3} \text{CNOT}_{0,1}) , \text{ for odd } n, \quad (9)$$

where w are adjustable parameters, and $\text{CNOT}_{m,n}$ represents CNOT gate with m as the control qubit and n as the target qubit. This particular way of circuit construction is plotted below in Figure 2 where b_i in the data encoding part of the second quantum circuit layer is the measured expectation value of σ_z

operator from qubit i of the previous quantum circuit layer.

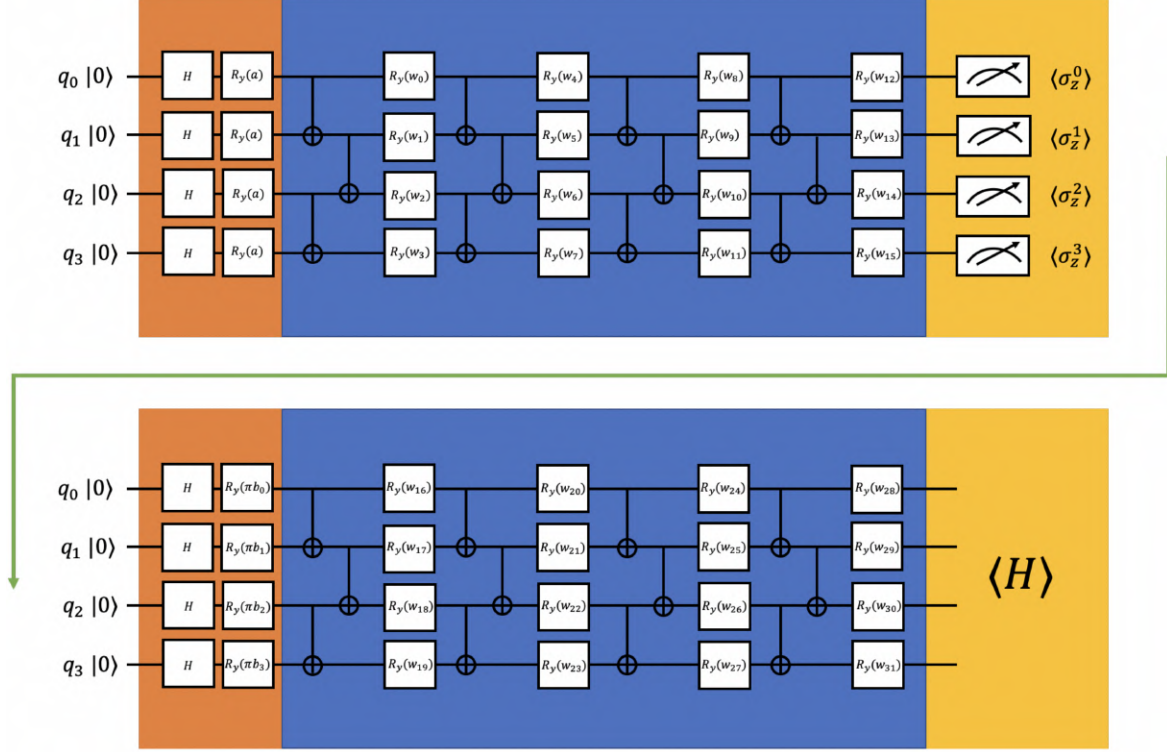


Figure 2: A 4-qubit quantum-classical neural network. The orange parts are data encoding, the blue parts are the variational (parametrized) quantum circuits, and the yellow parts are measurements. Notice that the first set of the measurements serve as nonlinear operations connecting the two PQCs. From [6].

Notice that the ways of arranging different gates and the numbers of qubits, repetition circuit units and circuit layers are not definite (i.e. there remains wide possibility and freedom for the construction of our hybrid neural network). For instance, we can adjust the types of the parameterized gates and the number of repetition units in our variational circuit (4 repetitions for the case in Figure 2), which would in turn affect our model expressibility and entangling capability.

(4) The Noise Model

To take the effect of quantum noise into consideration, we will investigate the performance of quantum simulations under noisy quantum computer configurations instead of running on noise-free simulator, which is more realistic to a NISQ [13] device. We will then implement the linear zero-noise extrapolation method for error mitigation [17, 4, 18].

2. 研究步骤

(1) Review previous researches regarding molecular Hamiltonian encoding (espe-

cially the Daubechies wavelet method) as well as quantum-classical hybrid neural networks, in order to come up with the research methods for this work.

- (2) Get familiar with the algorithm flow of Variational Quantum Eigensolver and modify several parts within it to adapt to the hybrid neural network method.
- (3) Calculate each term of the Hamiltonian of chosen molecules (e.g. H_2 , LiH , H_2O) by performing a Hartree-Fock calculation using the BigDFT code [11, 19], an *ab initio* software package that employs Daubechies wavelet basis sets. Then, select a minimal number of spin orbitals from the BigDFT output to form a set of (minimal) basis Daubechies wavelet molecular orbitals for the subsequent quantum simulations.
- (4) Train the proposed hybrid quantum-classical neural network on several indicated bond lengths.
- (5) Apply the rest of the bond lengths to the trained network as input with error mitigation techniques applied to the output.
- (6) Conduct experiments and get the potential energy surface of various small molecules to evaluate the accuracy and efficiency of our method and compare with previous works.
- (7) Fine-tune our works and conduct academic paper writing.

(五) 預期結果

1. Performance

As mentioned in (二), there are several crucial indicators to evaluate the work, including the deviation between the generated ground state energy surface and the experimental results, the circuit size, the runtime and qubit used during model generation and simulation calculations.

For chemical accuracy, since the Daubechies wavelet basis orbitals possess advantageous features over those of other basis sets (e.g. STO-3G or 6-31G), the self-consistent field calculations based on a Daubechies wavelet basis set can prepare a better set of molecular orbitals, which in turn results in a better many-body Hamiltonian. Thus it is expected that the accuracy of our model will be comparable with or even better than previous works.

For circuit size, since we will conduct tests on a variety of quantum neural network architecture in this research, it is expected to result in a resource-efficient and short-depth circuit while maintaining the desired chemical accuracy.

2. Novelty

Though several previous researches in quantum computational chemistry areas which took neural-network-based approaches had overcome some bottlenecks of the corresponding VQE algorithm flows [20, 21] for calculating molecular potential energy

surfaces, it's unprecedented to apply quantum machine learning methods into quantum computational chemistry with molecular Hamiltonian generated by Daubechies wavelet orbital basis. It is thus expected that this work could break the bottleneck of finding more accurate molecular properties and would even develop a new series of systematical methods in relevant research areas.

(六) 参考文献

- [1] Alberto Peruzzo et al. "A variational eigenvalue solver on a photonic quantum processor". In: *Nature communications* 5.1 (2014), pp. 1–7.
- [2] Jarrod R McClean et al. "The theory of variational hybrid quantum-classical algorithms". In: *New Journal of Physics* 18.2 (2016), p. 023023.
- [3] Sam McArdle et al. "Quantum computational chemistry". In: *Review of Modern Physics* 92.1 (2020), p. 015003.
- [4] Yu Shee et al. "A Qubit-Efficient Encoding Scheme for Quantum Simulations of Electronic Structure". In: *arXiv preprint arXiv:2110.04112* (2021).
- [5] Cheng-Lin Hong et al. "Accurate and efficient quantum computations of molecular properties using Daubechies wavelet molecular orbitals: a benchmark study against experimental data". 2021.
- [6] Rongxin Xia and Sabre Kais. "Hybrid quantum-classical neural network for calculating ground state energies of molecules". In: *Entropy* 22.8 (2020), p. 828.
- [7] Attila Szabo and Neil S Ostlund. *Modern quantum chemistry: introduction to advanced electronic structure theory*. Courier Corporation, 2012.
- [8] Trygve Helgaker, Poul Jorgensen, and Jeppe Olsen. *Molecular electronic-structure theory*. John Wiley & Sons, 2014.
- [9] Stephan Mohr et al. "Accurate and efficient linear scaling DFT calculations with universal applicability". In: *Physical Chemistry Chemical Physics* 17.47 (2015), pp. 31360–31370.
- [10] Laura E Ratcliff et al. "Flexibilities of wavelets as a computational basis set for large-scale electronic structure calculations". In: *The Journal of chemical physics* 152.19 (2020), p. 194110.
- [11] Luigi Genovese et al. "Daubechies wavelets as a basis set for density functional pseudopotential calculations". In: *The Journal of chemical physics* 129.1 (2008), p. 014109.
- [12] Jonathan Romero and Alán Aspuru-Guzik. "Variational quantum generators: Generative adversarial quantum machine learning for continuous distributions". In: *Advanced Quantum Technologies* 4.1 (2021), p. 2000003.
- [13] John Preskill. "Quantum computing in the NISQ era and beyond". In: *Quantum* 2 (2018), p. 79.
- [14] Qiming Sun et al. "PySCF: the Python-based simulations of chemistry framework". In: *Wiley Interdisciplinary Reviews: Computational Molecular Science* 8.1 (2018), e1340.
- [15] Jarrod R McClean et al. "OpenFermion: the electronic structure package for quantum computers". In: *Quantum Science and Technology* 5.3 (2020), p. 034014.

- [16] Sukin Sim, Peter D Johnson, and Alán Aspuru-Guzik. “Expressibility and entangling capability of parameterized quantum circuits for hybrid quantum-classical algorithms”. In: *Advanced Quantum Technologies* 2.12 (2019), p. 1900070.
- [17] Tudor Giurgica-Tiron et al. “Digital zero noise extrapolation for quantum error mitigation”. In: *2020 IEEE International Conference on Quantum Computing and Engineering (QCE)*. IEEE. 2020, pp. 306–316.
- [18] Ryan LaRose et al. “Mitiq: A software package for error mitigation on noisy quantum computers”. In: *arXiv preprint arXiv:2009.04417* (2020).
- [19] Stephan Mohr et al. “Daubechies wavelets for linear scaling density functional theory”. In: *The Journal of chemical physics* 140.20 (2014), p. 204110.
- [20] Rongxin Xia and Sabre Kais. “Quantum machine learning for electronic structure calculations”. In: *Nature communications* 9.1 (2018), pp. 1–6.
- [21] Kelvin Ch’Ng et al. “Machine learning phases of strongly correlated fermions”. In: *Physical Review X* 7.3 (2017), p. 031038.

(七) 需要指導教授指導內容

1. **Discussion about the direction of the research:** It’s my first time engaging in such an academic research, so I’m not familiar with the whole process of conducting a research. Through regular meeting with Prof. Goan, I can avoid getting lost during the research.
2. **Clarification of the Daubechies wavelet method and quantum neural network architecture:** Prof. Goan is an expert in quantum computing and possesses extensive research experiences about the topics of quantum computational chemistry and quantum machine learning. The methods in this work could be justified with the help of Prof. Goan.
3. **Usage of relevant software packages (e.g. IBM Qiskit, OpenFermion):** This research is based on the quantum machine simulator IBM qiskit package, which Prof. Goan possess extensive experience manipulating with.

三、耗材、物品、圖書及雜項費用：

- (一) 凡執行研究計畫所需之耗材、物品、圖書及雜項費用，均可填入本表內。
 (二) 說明欄請就該項目之規格、用途等相關資料詳細填寫，以利審查。
 (三) 依研究計畫實際需求擇優補助，每一計畫最高以補助新臺幣 20,000 元為限。

金額單位：新臺幣元

項 目 名 稱	說明	單位	數量	單價	金額	備註
Nielsen, M., & Chuang, I. (2010). Quantum Computation and Quantum Information: 10th Anniversary Edition. Cambridge: Cambridge University Press.	Acquire basic knowledge of quantum computation and quantum information from one of the most cited books in physics of all time. This comprehensive textbook describes such remarkable effects as fast quantum algorithms, quantum teleportation, quantum cryptography and quantum error-correction.	本	1	2102	2102	
Taku Onishi. Quantum Computational Chemistry: Modelling and Calculation for Functional Materials (ISBN-13: 978-9811355288)	This book is for both theoretical and experimental chemists to begin quantum molecular orbital calculations for functional materials. First, the theoretical background including the molecular orbital calculation method and modelling are explained, followed by an explanation of how to do modelling and calculation and to interpret calculated molecular orbitals.	本	1	3719	3719	
Typora	A minimal Markdown editor and reader, which is using GitHub flavored markdown. Typora supports export to current document into PDF, HTML, HTML (without styles) and Image format.	套	1	415	415	
雜支	包括文具, 紙張, 影印, 論文郵寄等作業。	/	/	/	2000	
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表 C803

國立臺灣大學學生歷年成績表

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學院名稱	理學院					畢業年月	
系組名稱	物理學系		輔系系組				
雙修系組			跨域專長				
課 號	科 目 名 稱	學 分	成 績	課 號	科 目 名 稱	學 分	成 績
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FL 1004 英文二	3	免修		Phys 3004 量子物理下			
PE 1003 健康體適能	1	抵免		Phys 3009 近代物理學實驗			
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MATH 1202 微積分甲下	4	抵免		Phys 2011 電子學二			
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Phys 1007 普通物理學甲下	3	抵免		Phys 8049 量子計算與資訊導論			
Phys 1026 普通物理學實驗上	1	抵免		修習學分：19.00 實得學分：19.00 學期GPA：4.25			
Phys 1027 普通物理學實驗下	1	抵免		109學年度第1學期			
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Chem 1006 普通化學甲下	3	抵免		PE 2064 羽球初級			
Chem 1011 普通化學實驗上	1	抵免		AdvEng 4013 線上學術英語一			
Chem 1012 普通化學實驗下	1	抵免		Phys 8050 量子計算與量子資訊專題			
MD&PH 5002 藝術概論一	2	抵免		Phys 8146 量子計算的應用場景			
107學年度第1學期				Phys 5052 量子光學導論			
AdvEng 2007 進階英語一	0	免修		CSIE 5432 機器學習基石			
Phys 1001 服務學習一	0	通過		CSIE 5433 機器學習技法			
Phys 2002 應用數學二	3	A+		修習學分：15.00 實得學分：15.00 學期GPA：4.26			
Phys 2004 力學上	3	A+		109學年度第2學期			
Phys 2017 力學習題演練上	1	A+		LING 5505 程式設計與資料科學導論			
Phys 2019 電磁學上	3	A+		EE 4052 計算機程式設計			
Phys 2021 電磁學習題演練上	1	A+		GenEdu 5005 C/C++程式設計			
Phys 3006 熱物理	3	A+		GenEdu 5006 Python 計算機程式設計			
Phi 1413 中國哲學導論	3	A+		GenEdu 5011 程式設計與資料分析			
CHIN 1031 中國傳統生命禮俗	2	A+		AdvEng 4014 線上學術英語二			
NtlDev 1093 全球通識講座：我國如何因應全球科技發展趨勢？	2	A+		BICD 1022 統計學與實習			
MD&PH 5008 現代生物技術與健康	2	A+		EE 1003 計算機概論			
Phys 1037 程式設計和物理模擬	2	A+		EE 5184 機器學習			
修習學分：25.00 實得學分：25.00 學期GPA：4.30				修習學分：25.00 實得學分：25.00 學期GPA：4.26			
107學年度第2學期				(以下空白)			
AdvEng 2008 進階英語二	0	免修					
CHIN 1082 大學國文二	3	A+					
PE 2064 羽球初級	1	A-					
Phys 2001 應用數學一	3	A+					
Phys 2005 力學下	3	A+					
Phys 2018 力學習題演練下	1	A+					
Phys 2020 電磁學下	3	A+					
Phys 2022 電磁學習題演練下	1	A+					
Phys 3001 應用數學三	3	A					
Phys 1039 國際學伴之服務學習	2	A+					
CSIE 1920 計算機概論	2	A+					
修習學分：22.00 實得學分：22.00 學期GPA：4.23							
108學年度第1學期							
PE 2064 羽球初級	1	A					
Phys 1002 服務學習二	0	通過					
Phys 1003 服務學習三	0	通過					
Phys 3003 量子物理上	4	A+					
Phys 3007 基礎物理實驗	3	A+					
Phys 1041 給未來首席執行長的物理學	2	A+					
Phys 1036 粒子物理的世界	2	A+					
ME 4116 現代科技與人類文明	2	A+					
Phys 2009 電子學一	3	A+					
ApPhys 7005 半導體導論	3	A+					
EE 2021 工程數學-微分方程(一)	2	A+					
EE 4036 電子電路設計	(3)	停修					
備 註							
實得總學分 162.00				註冊組主任 李宏棟			
修習及格學分 129.00	抵免學分 27.00	免修學分 6.00	暑修學分 0.00	採計學分 0.00			

印製日期：110年09月01日

單科成績對應績分：A+=4.3 A=4.0 A-=3.7 B+=3.3 B=3.0 B-=2.7 C+=2.3 C=2.0 C-=1.7 F=0 X=0

第1之1頁

國立臺灣大學成績單說明

壹、評分標準

一、本校於 99 學年度以前，採用百分制方式評量學生成績，其標準如下：

學士班成績	等第制成績	研究生成績
80 分以上	A	80 分以上
70-79 分	B	70-79 分
60-69 分	C	69 分以下
50-59 分	D	
49 分以下	E	
備註：70 分為研究生及格標準；60 分為學士班及格標準		

二、本校於 99 學年度（含）以後，採用等第制方式評量學生成績，其標準如下：

等第制成績	定義	等第績分	對照百分制分數區間
A+	所有目標皆達成且超越期望	4.3	90-100 分
A	所有目標皆達成	4.0	85-89 分
A-	所有目標皆達成，但需一些精進	3.7	80-84 分
B+	達成部分目標，且品質佳	3.3	77-79 分
B	達成部分目標，但品質普通	3.0	73-76 分
B- (研究生及格標準)	達成部分目標，但有些缺失	2.7	70-72 分
C+	達成最低目標	2.3	67-69 分
C	達成最低目標，但有些缺失	2.0	63-66 分
C- (學士班及格標準)	達成最低目標但有重大缺失	1.7	60-62 分
F	未達成最低目標	0	59 分(含)以下
X	因故不核予成績	0	0
W	停修		
NG	成績未到		
IP	撰寫論文		
TR	抵免		
EX	免修		

貳、課號編碼規則

一、課號由「開課單位英文縮寫」及 4 碼「基本課號」組成。

二、開課單位英文縮寫請見本校網址：http://www.aca.ntu.edu.tw/curri/curs_deptabb.asp

NATIONAL TAIWAN UNIVERSITY TRANSCRIPT GUIDE

GRADING SYSTEM :

1、The numerical grading system was in effect PRIOR TO SEPTEMBER 2010 :

Undergraduate Programs	Letter Grades	Graduate Programs
80 AND ABOVE	A	80 AND ABOVE
70-79	B	70-79*
60-69**	C	69 AND BELOW
50-59	D	
49 AND BELOW	E	
* For the graduate students, the passing grade is 70.		
** For the undergraduate students, the passing grade is 60.		

2、EFFECTIVE SEPTEMBER 2010, the following letter grading system appears on transcripts :

Letter Grading System	Definition	Grade Points	Conversion Scale
A+	All goals achieved beyond expectation	4.3	90-100
A	All goals achieved	4.0	85-89
A-	All goals achieved, but need some polish	3.7	80-84
B+	Some goals well achieved	3.3	77-79
B	Some goals adequately achieved	3.0	73-76
B- (passing grade for graduate students)	Some goals achieved with minor flaws	2.7	70-72
C+	Minimum goals achieved	2.3	67-69
C	Minimum goals achieved with minor flaws	2.0	63-66
C- (passing grade for undergraduate)	Minimum goals achieved with major flaws	1.7	60-62
F	Minimum goals not achieved	0	50 AND BELOW
X	Not graded due to unexcused absences or withdrawal	0	0
W	No grade reported		
NG	In progress		
IP	Transfer credit		
TR	Exempted		
EX			

COURSE NUMBERS :

1、Course numbers are 4-digit basic numbers prefixed with abbreviated department names.

2、For the department abbreviation, please refer to the university website at http://www.aca.ntu.edu.tw/curri/curs_deptabb_e.asp