NOISY QUANTUM COMPUTING OF ELECTRONIC STRUCTURE OF CRYSTALS

[1,2]Vojtěch VAŠINA, [2]Ivana MIHÁLIKOVÁ, [2]Martin FRIÁK

[1]Brno University of Technology, Faculty of Mechanical Engineering, Institute of Materials Science and Engineering, Brno, Czech Republic, EU, vasina@ipm.cz

[2]Institute of Physics of Materials, v.v.i., Czech Academy of Sciences, Brno, Czech Republic, EU, mihalikova@ipm.cz, friak@ipm.cz

https://doi.org/10.37904/metal.2025.5153

Abstract

Quantum computing is currently emerging as a useful paradigm for solving highly complex computational problems. Current quantum computers are unfortunately too noisy to provide sufficient accuracy, and quantum-classical hybrid algorithms emerged as a solution. Variational Quantum Deflation (VQD) has gained significant attention for addressing challenges in quantum chemistry, material science, etc. VQDs typically use multiple optimization methods, and the correct choice of optimization method can significantly impact performance. In our study, we focused on the comparison of multiple optimization methods used in VQD when applied to the electronic structure of crystals. The quantum part of VQD ran on a classical simulator with imported noise models from real quantum computers from the IBM Quantum Platform.

Keywords: Quantum computers, optimization methods, variational quantum deflation (VQD), hybrid quantum computing, impact of noise

1. INTRODUCTION

Accurately knowing the electronic band structure of a crystal is very important in computational material science, because many physical properties can be derived from the electronic band structure. However, the problem of computing the band structure with classical computers can become significantly more computationally demanding as the system grows in size. Today's most powerful supercomputers are not capable of simulating more than several hundreds or thousands of atoms.

Quantum computers are emerging as a potential solution to this problem thanks to their capability to solve certain problems much faster than classical computers. Since quantum computers are relatively new technology and quantum states of qubits are vulnerable to the surrounding environment, the quantum computers can be significantly affected by noise. As a solution to this problem, hybrid classical-quantum algorithms are used, combining computations on the quantum computers with classical computers.

In our study we used Variational Quantum Deflation (VQD) [1] algorithm to compute electronic band structure of the silicon crystal following the study of M. Ďuriška [2]. Our goal was to include the noise model of a real quantum computer to the calculations and to study how the results will be affected. We also studied how many iterations of the classical optimization method are required in order to achieve satisfactory results. The results obtained from VQD algorithm were compared with electronic band structure obtained as a classical solution of the tight binding method [3]. Noise model included in calculations has been imported from the real quantum computer from IBM Quantum Platform [4].

2. HAMILTON OPERATOR OF THE SYSTEM

In order to compute the band structure of any crystal it is required to know its Hamilton operator which determines the total energy of the physical system [5]. The eigenvalues of the Hamilton operator are energy levels of the system [6]. The Hamilton operator of silicon for our study has been obtained from study of M. Ďuriška [2] and it is specified by the following matrix:

$$\hat{H} = \det \begin{bmatrix} E_s & V_{ss}g_0 & 0 & 0 & 0 & V_{sp}g_1 & V_{sp}g_2 & V_{sp}g_3 \\ V_{ss}g_0^\dagger & E_s & -V_{sp}g_1^\dagger & -V_{sp}g_2^\dagger & -V_{sp}g_3^\dagger & 0 & 0 & 0 \\ 0 & -V_{sp}g_1 & E_p & 0 & 0 & V_{xx}g_0 & V_{xy}g_3 & V_{xy}g_1 \\ 0 & -V_{sp}g_2 & 0 & E_p & 0 & V_{xy}g_3 & V_{xx}g_0 & V_{xy}g_1 \\ 0 & -V_{sp}g_3 & 0 & 0 & E_p & V_{xy}g_1 & V_{xy}g_2 & V_{xy}g_0 \\ V_{sp}g_1^\dagger & 0 & V_{xx}g_0^\dagger & V_{xy}g_3^\dagger & V_{xy}g_1^\dagger & E_p & 0 & 0 \\ V_{sp}g_2^\dagger & 0 & V_{xy}g_3^\dagger & V_{xx}g_0^\dagger & V_{xy}g_0^\dagger & 0 & E_p & 0 \\ V_{sp}g_3^\dagger & 0 & V_{xy}g_1^\dagger & V_{xy}g_1^\dagger & V_{xx}g_0^\dagger & 0 & 0 & E_p \end{bmatrix} \quad (1)$$

where: E_s = -4.03 eV, E_p = 3.17 eV, V_{ss} = -8.13 eV, V_{sp} = 5.88 eV, V_{xx} = 3.17 eV, V_{xy} = 7.51 eV are energies obtained from [7], $g_0^\dagger$, $g_1^\dagger$, $g_2^\dagger$, $g_3^\dagger$ are Hermitian transposed vectors g_0, g_1, g_2, g_3 defined as:

$$g_0(\vec{k}) = \frac{1}{4}(e^{i\vec{k}\vec{d_0}} + e^{i\vec{k}\vec{d_1}} + e^{i\vec{k}\vec{d_2}} + e^{i\vec{k}\vec{d_3}}) \ , \ g_1(\vec{k}) = \frac{1}{4}(e^{i\vec{k}\vec{d_0}} + e^{i\vec{k}\vec{d_1}} - e^{i\vec{k}\vec{d_2}} - e^{i\vec{k}\vec{d_3}})$$

$$g_2(\vec{k}) = \frac{1}{4}(e^{i\vec{k}\vec{d_0}} - e^{i\vec{k}\vec{d_1}} + e^{i\vec{k}\vec{d_2}} + e^{i\vec{k}\vec{d_3}}) \ , \ g_3(\vec{k}) = \frac{1}{4}(e^{i\vec{k}\vec{d_0}} - e^{i\vec{k}\vec{d_1}} - e^{i\vec{k}\vec{d_2}} - e^{i\vec{k}\vec{d_3}}) \quad (2)$$

where the $\vec{k}$ - vector defines the position in which Hamilton operator is determined and $\vec{d}_0, \vec{d}_1, \vec{d}_2, \vec{d}_3$ are positions of the closest atoms relative to the atom located at (0,0,0), in particular

$$\vec{d}_0 = \frac{a}{4}(1,1,1); \quad \vec{d}_1 = \frac{a}{4}(1,-1,-1); \quad \vec{d}_2 = \frac{a}{4}(-1,1,-1); \quad \vec{d}_3 = \frac{a}{4}(-1,-1,1) \quad (3)$$

where *a* is the lattice parameter of silicon obtained from [8] and equal to *a* = 0.543 nm.

3. METHODS

3.1 Variational Quantum Deflation (VQD)

To compute *k* lowest eigenvalues of the Hamiltonian given by matrix (1), the Variational Quantum Deflation (VQD) has been chosen. The *k*-th eigenvalue, i.e. the *k*-th energy level, is obtained by finding the minimum of the cost function for the respective eigenvalue. The cost function has been specified by Higgott [1]:

$$C_k(\vec{\theta}) = \langle\psi(\vec{\theta})|\hat{H}|\psi(\vec{\theta})\rangle + \sum_{i=0}^{n-1}\beta_i|\langle\psi(\vec{\theta})|\hat{H}|\psi(\vec{\theta}_i)\rangle|^2 \quad (4)$$

where $\vec{\theta}$ I the vector of variational parameters, which can be changed in order to minimize the cost function, $\vec{\theta}_i$ is the vector of parameters resulting from minimization of the cost function for the *n*-1-th eigenvalue and β_i parameters represent an overlap and should be higher than $E_{i+1} - E_i \geq \beta_i$. After each evaluation of the cost function the results are post processed.

3.2 Classical optimization method

Classical optimization is a key component of variational quantum algorithms. The optimization routine is used to minimize the cost function, given by the Equation 4, by iteratively adjusting components of the vector $\vec{\theta}$. For our study we employed the Constrained Optimization by Linear Approximation (COBYLA) method, because from experiments conducted by Bonet-Monroig *et al.* [9] the COBYLA resulted as a reasonable compromise between speed and accuracy. Another reason for choosing COBYLA is its universality as it can be used for noiseless and noisy environments. By choosing the same optimization method for noiseless and noisy environments we can directly compare the results for both scenarios.

COBYLA is a derivative-free optimization algorithm, defined by Powell [10], which operates by constructing linear approximations to the objective function within a trust region framework, making it robust against measurement noise and the non-smooth nature of quantum cost landscapes. Its effectiveness in our simulations underscores the importance of selecting appropriate classical optimizers in variational quantum computing, especially when operating under realistic noise conditions. The choice of optimizer can significantly influence convergence behaviour and solution quality, and thus remains a critical factor in the overall performance of hybrid quantum-classical algorithms.

3.3 Variational form

Another critical element of the variational quantum algorithm is an appropriately chosen ansatz. The ansatz is a parametrized quantum circuit [11] used to approximate the eigenstates of the Hamiltonian. The structure of ansatz can significantly influence the quality of final results and also speed of the algorithm. For the case of our study the *EfficientSU2* ansatz has been chosen as provided by *Qiskit Circuit Library* [12]. The ansatz has been designed as a 3 qubit quantum circuit with 24 parametrized quantum gates, see **Figure 1**. Each qubit in the circuit has been entangled with all other qubits in the circuit, this type of entanglement is typically called full entanglement.

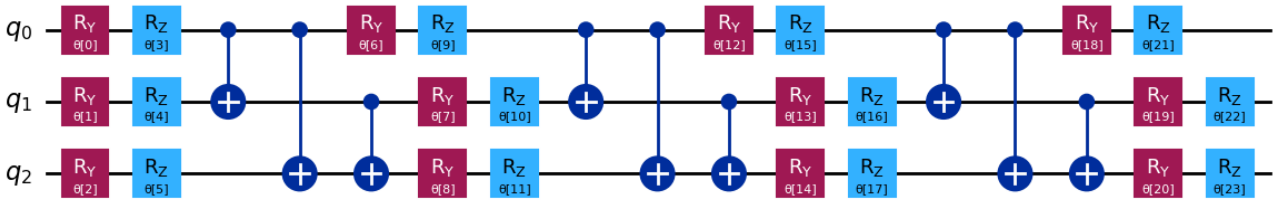


Figure 1 A schematic visualization of the used ansatz EfficientSU2.

4. RESULTS

To highlight the impact of noise on the accuracy, computations were conducted for four different iteration counts e.g. 100, 1000, 5000 and 10000. Each iteration count has been tested under two scenarios: (i) on the simulator of ideal quantum computer, without any noise, and (ii) on the simulator of real quantum computer with imported noise model from IBM Quantum Platform. The noise model has been imported from device ibm_brisbane which possesses quantum processor Eagle r3 with 127 qubits based on superconducting technology [4]. Number of *k*-points for the results including the effect of noise has been reduced in order to save computational resources. Results without the noise are plotted on **Figure 2** (100 iterations), **Figure 4** (1000 iterations), **Figure 6** (5000 iterations), **Figure 8** (10000 iterations), see below. Results that include the effects of noise are plotted on **Figure 3** (100 iterations), **Figure 5** (1000 iterations), **Figure 7** (5000 iterations), **Figure 9** (10000 iterations), see below.

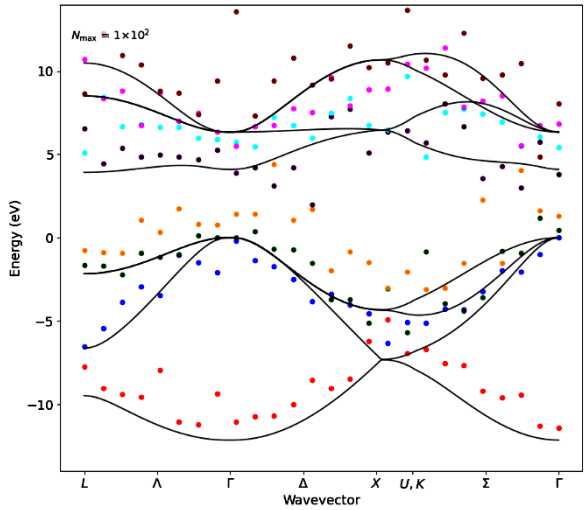


Figure 2 Band structure after 100 iterations

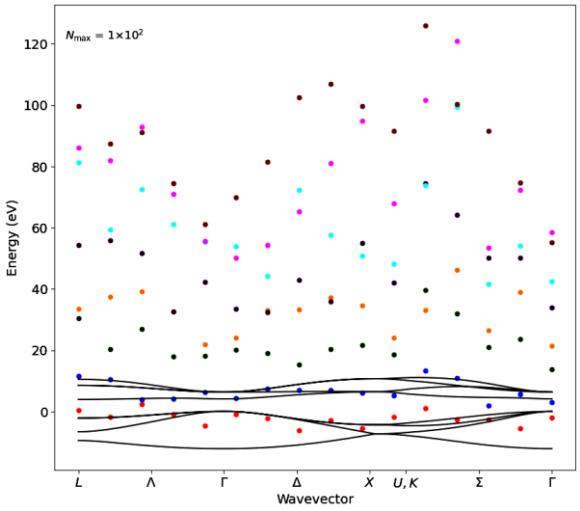
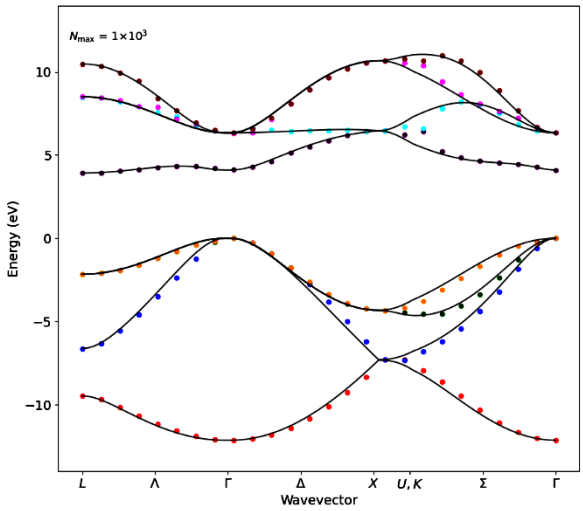
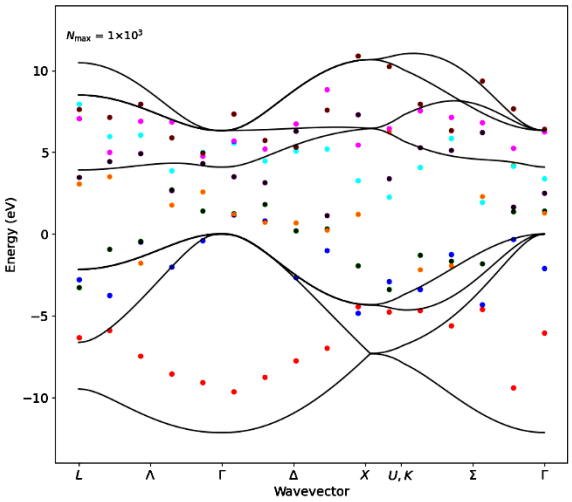


Figure 3 Band structure after 100 iterations,





noise included

Figure 4 Band structure after 1000 iterations

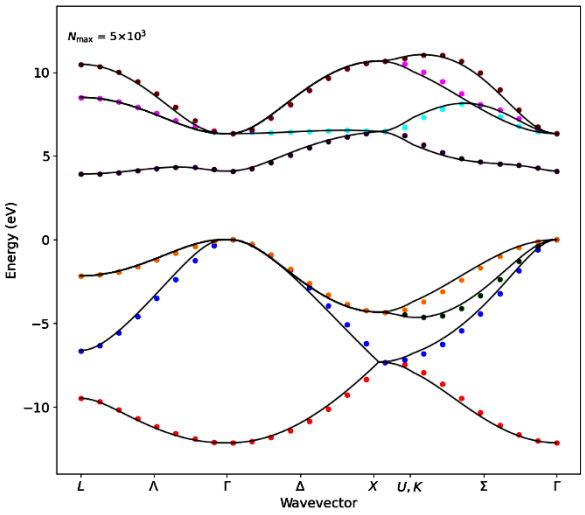


Figure 5 Band structure after 1000 iterations, noise included

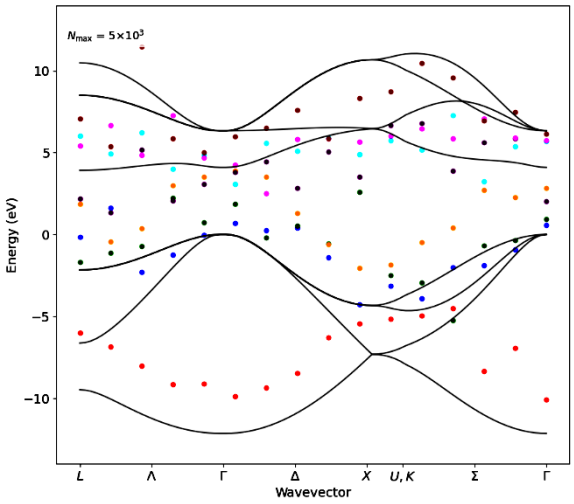


Figure 6 Band structure after 5000 iterations

Figure 7 Band structure after 5000 iterations, noise included

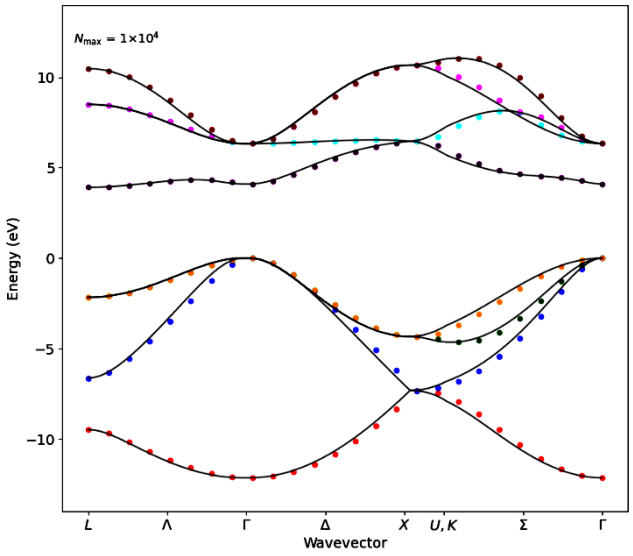


Figure 8 Band structure after 10000 iterations

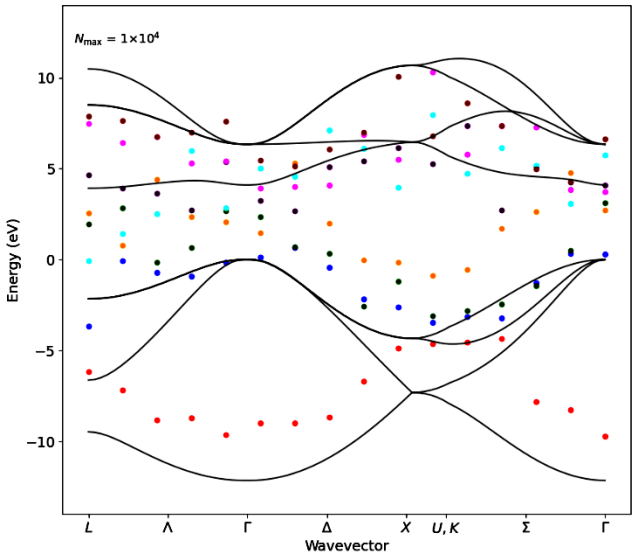


Figure 9 Band structure after 10000 iterations, noise included

5. CONCLUSION

In our study, we explored the feasibility of computing electronic band structure using simulators of the quantum computers. Two distinct strategies were incorporated: simulations without noise, which represented an ideal quantum computer, and simulations with imported noise models simulating a real quantum device. The VQD algorithm has been executed with both strategies with and without the effects of noise.

Results from the noiseless simulations demonstrated that VQD algorithm can be successfully implemented to compute electronic band structure of the crystal described by Hamiltonian. From the results it is also clear that results are becoming more accurate as the number of iterations increases, i. e. with accordance with the studies such as Refs. [2, 13]. Noiseless results obtained from our computations show a strong agreement with electronic band structure obtained using classical computers.

The results with included noise model represent capabilities of the current commercially available quantum computers. Unfortunately, a significant degradation in accuracy and increased variance of the results was found. Our results highlight the sensitivity of quantum algorithms to decoherence and quantum gate errors. Even under noisy conditions some quantitative aspects of the band structure remained distinguishable, suggesting that error-mitigation and error-correction strategies could be used to enhance the quality of the results.

Our study highlights the current promises and present-day limitations of quantum computing in the context of computational material science. We demonstrate that while quantum algorithms are capable of capturing essential physical characteristics, their practical deployment remains constrained by the imperfections of current hardware. As the quantum computers and error-correction algorithms continue to evolve we anticipate that simulation of the electronic band structure will become not only practical but advantageous over classical computational methods in near future. This is expected to be especially true for complex systems where classical computational methods face scalability challenges.

ACKNOWLEDGEMENTS

Financial supports from the Czech Academy of Science are gratefully acknowledged, in particular the Praemium Academiae awarded to Mgr. Martin Friák, Ph.D., and the Strategy AV21 (the program "AI:

Artificial Intelligence for Science and Society"). The computational resources were partly provided by the Ministry of Education, Youth and Sports of the Czech Republic under the Project e-INFRA CZ (ID:90254) at the IT4Innovations National Supercomputing Center, the MetaCentrum and CERIT-SC. Access to the CERIT-SC computing and storage facilities provided by the CERIT-SC Center, under the programme "Projects of Large Research, Development, and Innovations Infrastructures" (CERIT Scientific Cloud LM2015085) and access to CESNET storage facilities provided by the project "e-INFRA CZ" under the programme "Projects of Large Research, Development, and Innovations Infrastructures" LM2023054) is acknowledged, and partly also by the IBM at the IBM Quantum Platform infrastructure.

REFERENCES

[1] HIGGOTT, O., WANG. D., BRIELEY, S. Variational quantum computation of excited states. *Quantum*. 2019, vol. 3, pp. 156 – 166.

[2] ĎURIŠKA, M. *Calculation of band structure by variational quantum methods.* Brno 2024, Diploma thesis. Masaryk University.

[3] ELSTNER, M., SEFERT, G. Density functional tight binding. *The Royal Society Publishing.* 2014, vol. 372, DOI: 2012.0483.

[4] IBM Quantum Platform, *Compute Resources.* [online]. 2025 [viewed:2025-05-10]. Available from: https://quantum.ibm.com/services/resources.

[5] STEFANUCCI, G. *Quantum Mechanics for Material Science,* Cham: Springer, 2024.

[6] ZETTILI, N. *Quantum Mechanics- Concepts and Applications,* Chichester: Wiley, 2009.

[7] CHADI, D.J., COHEN, M.L., Tight-binding calculations of the valence bands of diamond and zincblende crystals, *Basic Solid State Physics.* 1975, vol. 68, pp. 405-419.

[8] The NIST Reference on Constants, Units, and Uncertainty, *Fundamental Physical Constants.* [online]. 2025 [viewed:2025-05-10]. Available from: https://physics.nist.gov/cgi-bin/cuu/Value?asil.

[9] BONET-MONROIG, X., WANG, H., VERMETTEN, D., SENJEAN, B., MOUSSA, Ch., BÄCK, T., DUNKJO, V., O'BRIEN, T.E. Performance comparison of optimization methods on variational quantum algorithms. *Physical Review A.* 2023, vol. 107, pp. 032407. doi: 107.032407.

[10] POWELL, M.J.D., Direct search algorithms for optimization calculations. *Acta Numerica*. 1998, vol. 7, pp. 287-336. doi:10.1017/S0962492900002841.

[11] IBM Quantum Learning, *Ansatze and Variational Forms.* [online]. 2025 [viewed:2025-05-12]. Available from: https://learning.quantum.ibm.com/course/variational-algorithm-design/ansatze-and-variational-forms.

[12] IBM Quantum Documentation. *EfficientSU2.* [online]. 2025. [viewed:2025-05-10]. Available from: https://docs.quantum.ibm.com/api/qiskit/qiskit.circuit.library.EfficientSU2.

[13] CERASOLI, F.T., SHERBERT, K., SLAWINSKA, J., NARDELLI, M.B., Quantum computation of silicon electronic band structure. *Physical Chemistry Chemical Physics.* 2020, vol.22, p. 21816.