QUANTUM-COMPUTING STUDY OF THE ELECTRONIC STRUCTURE OF CRYSTALS: THE CASE STUDY OF SI

[1,2]Michal ĎURIŠKA, [1,2]Ivana MIHÁLIKOVÁ, [1,2]Martin FRIÁK

[1]*Institute of Physics of Materials, v.v.i., Czech Academy of Sciences, Brno, Czech Republic, EU,* *484267@mail.muni.cz; mihalikova@ipm.cz; friak@ipm.cz*

[2]*Institute of Solid State Physics, Faculty of Science, Masaryk University, Brno, Czech Republic, EU*

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Abstract

Quantum computing is newly emerging information-processing technology which is foreseen to be exponentially faster than classical supercomputers. Current quantum processors are nevertheless very limited in their availability and performance and many important software tools for them do not exist yet. Therefore, various systems are studied by simulating the run of quantum computers. Building upon our previous experience with quantum computing of small molecular systems (see I. Miháliková *et al*., Molecules 27 (2022) 597, and I. Miháliková *et al.*, Nanomaterials 2022, 12, 243), we have recently focused on computing electronic structure of periodic crystalline materials. Being inspired by the work of Cerasoli et al. (Phys. Chem. Chem. Phys., 2020, 22, 21816), we have used hybrid variational quantum eigensolver (VQE) algorithm, which combined classical and quantum information processing. Employing tight-binding type of crystal description, we present our results for crystalline diamond-structure silicon. In particular, we focus on the states along the lowest occupied band within the electronic structure of Si and compare the results with values obtained by classical means. While we demonstrate an excellence agreement between classical and quantum-computed results in most of our calculations, we further critically check the sensitivity of our results with respect to computational set-up in our quantum-computing study. A few results were obtained also using quantum processors provided by the IBM.

Keywords: Quantum computing, crystals, tight-binding method, quantum-mechanical calculations

1. INTRODUCTION

Quantum information emerged as a scientific field a few decades ago and managed to draw the attention of wide community due to several pioneering achievements. The newly emerging quantum-computers promise to be a revolutionary ground-breaking solution for future calculations. Probably the best-known application is the ability of quantum computers to efficiently find (prime) factors of large numbers, known as the Shor algorithm [1]. While a lot of attention is paid world-wide prime factorization, which is essential for the security of online communication, we will focus on application of quantum computers in physics where the situation is less understood and methodologically rather underdeveloped. In fact, for now it is far from clear, which is the most promising physical platform (trapped ions, optical lattices, …) for developing suitable quantum computers.

Currently, different companies from leaders in the IT market such as IBM [2] or Google [3] to newly emerging start-ups like Rigetti [4] work on their quantum computers mostly independently. In all cases, however, these devices are rather small (counting dozens of qubits) and rather noisy (with the error rate orders of magnitude larger than the one needed for efficient error correction). Last, but not least, these devices have a rather restricted connectivity between the qubits. This means that an operation on two distant part of the computer involves a long set of operation on neighboring qubits, leading to an inacceptable increase in errors. And while Google recently claimed its computer reached the so-called quantum supremacy [3], in some sense it is still

very far from being able to solve any problem that a simple scientific calculator cannot. Importantly, there is a tremendous progress in the development of new quantum algorithms [5] including those for solving sets of linear equations in general (see, e.g. that of Harrow, Hassidim and Lloyd [6]), or those which would optimize mixing of iterative methods [7].

Our work was motivated by recent applications of quantum computing in the field of solid states physics, see, e.g., Ref. [8]. Considering current difficulties when obtaining (access to) quantum computers, we have mostly simulated the run of a quantum processor. We focused on the dependence of the results on the number of use of the quantum part of the algorithm (number of iterations) in order to examine how sensitive the results are on these computational aspects and what is the minimum necessary number of iterations in order to obtained reliable results. Next, as a complement to our simulations, we have also obtained a few results from a physical realization of a quantum computer when employing IBM Quantum platform.

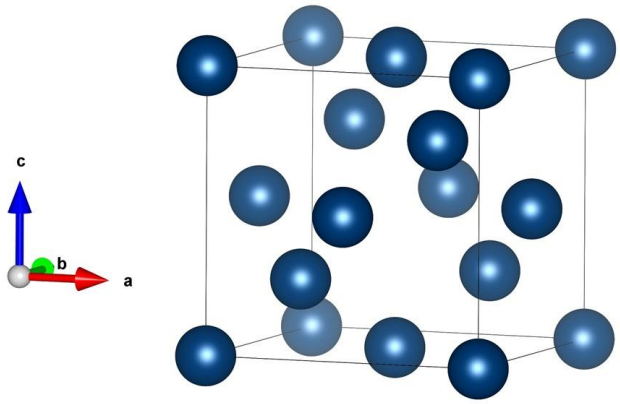

Figure 1 The diamond structure of Si (some atoms are shown with their periodically repeated images).

2. COMPUTATIONAL METHODOLOGY

Our calculations are based on the tight-binding method according to Slater and Koster [9] which was used when constructing a parametrized Hamiltonian $H(\boldsymbol{k})$. In case of Si, we have two atoms in the primitive unit cell that are tetrahedrally coordinated, see **Figure 1**. While four orbitals s, p_x, p_y, p_z centred around each atom site are usually considered, we simplified the simulation (for the sake of minimizing the use of the quantum resources) and we took into account only the interactions between s orbitals resulting in the Hamiltonian

$$H(\boldsymbol{k}) = \begin{pmatrix} E_s & g(\boldsymbol{k})V_{ss} \\ g(\boldsymbol{k})^* V_{ss} & E_s \end{pmatrix}, \tag{1}$$

where the matrix elements $E_s = -4.03\ \mathrm{eV}$ is on-site energy, $V_{ss} = -8.13\ \mathrm{eV}$ is hopping energy between s orbitals and $g(\boldsymbol{k})$ is given by

$$g(\boldsymbol{k}) = 1/4\left(e^{i\boldsymbol{k}.\boldsymbol{d_1}} + e^{i\boldsymbol{k}.\boldsymbol{d_2}} + e^{i\boldsymbol{k}.\boldsymbol{d_3}} + e^{i\boldsymbol{k}.\boldsymbol{d_4}}\right). \tag{2}$$

Vectors $\boldsymbol{d_1}, \boldsymbol{d_2}, \boldsymbol{d_3}, \boldsymbol{d_4}$ are positions of four nearest neighbors around atom at $[0,0,0]$. Numerical values of matrix elements E_s, V_{ss} were taken from [10]. Classically, the energy eigenvalues of this 2x2 matrix are given by

$$E(\boldsymbol{k}) = E_s \pm Vss|g(\boldsymbol{k})|, \tag{3}$$

resulting in two bands.

To simulate this model on quantum computer we must transform the Hamiltonian (1) to the qubit space. One such a mapping can be accomplished by expressing (1) in terms of Pauli matrices. Hermitian matrix (1) can be decomposed using the complete Pauli basis $\sigma = (I, X, Y, Z)$. For 2x2 matrices this is quite simple

$$H(\boldsymbol{k}) \rightarrow \sum_{j=I,X,Y,Z} c_j \sigma_j, \tag{4}$$

and the coefficients c_j are given by

$$c_j = \left(\frac{1}{4}\right) * \mathrm{Tr}(\sigma_j H(\boldsymbol{k})). \tag{5}$$

This mapping requires only one qubit.

Our calculations were performed using the Variational Quantum Eigensolver (VQE) [11]. It is an algorithmic method for finding the ground energy of a Hamiltonian using both classical and quantum computer. The advantage of this method, compared to other quantum algorithms for the same task (e.g. quantum phase estimation [12]) is that it uses only very shallow (small) quantum circuits, therefore it is suitable for noisy quantum computers – only a handful operations on each qubit are needed, therefore the amount of errors that accumulate on each qubit is not prohibitive.

In the VQE algorithm, the following cycle is being run till reaching the goal with a defined precision:

1. Preparation of a parametrized quantum state and select a probe point in the sample space
2. Measurement of each Hamiltonian term on the quantum devices
3. Calculation of the energy
4. Using a classical optimization method to adjust the point in the sample space
5. Return to point 2.

Depending on the nature of the problem, both adjusting the sample point and calculating the cost function might be very complicated. If we e.g. search for a ground state of the Hamiltonian, walking within the state space is rather easy. On the other hand, if we aim to get a large set of orthogonal vectors, finding a proper adjusted point might be computationally very costly.

For the preparation of parametrized quantum state we used the heuristic $R_y R_z$ variational form consisting of parametrized R_y and R_z single qubit rotations, see **Figure 2**. To estimate expectation values of the Hamiltonian terms, we used so-called post-rotations that allowed us to switch basis of the Hamiltonian terms from the non-diagonal basis to the diagonal ones. The optimization method used in our calculations is the Constrained Optimization by Linear Approximation (COBYLA) [13]. The calculations proceed iteratively with the maximum number of iterations (the parameter MAXITER) chosen by the user.

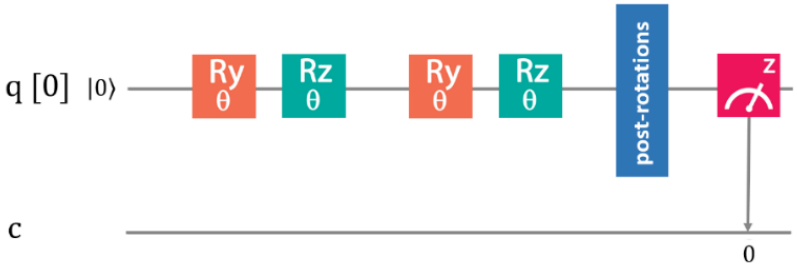

Figure 2 A schematics of the used quantum circuit.

3. RESULTS

A critical aspect related to the current use of quantum computers is that they are very limited as a computing resource. While several companies provide platforms, with some of them cost-free to use, the actual access to quantum computing resources is rather limited. It is therefore desirable to minimize the number of calls of quantum unit on one hand while obtaining results of an acceptable accuracy on the other, see, e.g. Ref. [14].

Figure 3 summarizes our results, i.e. energies within the two lowest occupied bands in the band structure of Si, for different number of iterations employing the VQE algorithm, defined by the MAXITER parameter, which are used when iteratively searching for the solution employing the COBYLA optimizing method. The results obtained when simulation the run of a quantum computer are visualized by blue circles and compared with results obtained by classical means (red curves). Analyzing the value of the MAXITER equal to 4, 6, 8, 10, 15 and 20, **Figure 3** clearly shows a trend when the results for low values of the MAXITER exhibit only very poor accuracy. A decent accuracy of the results is obtained only for increasing values of the MAXITER parameter, e.g. for MAXITER = 20 (and likely higher values). It is also apparent that the lower energies are reliably reproduced for lower values of MAXITER compared with the value needed for the higher-energy band.

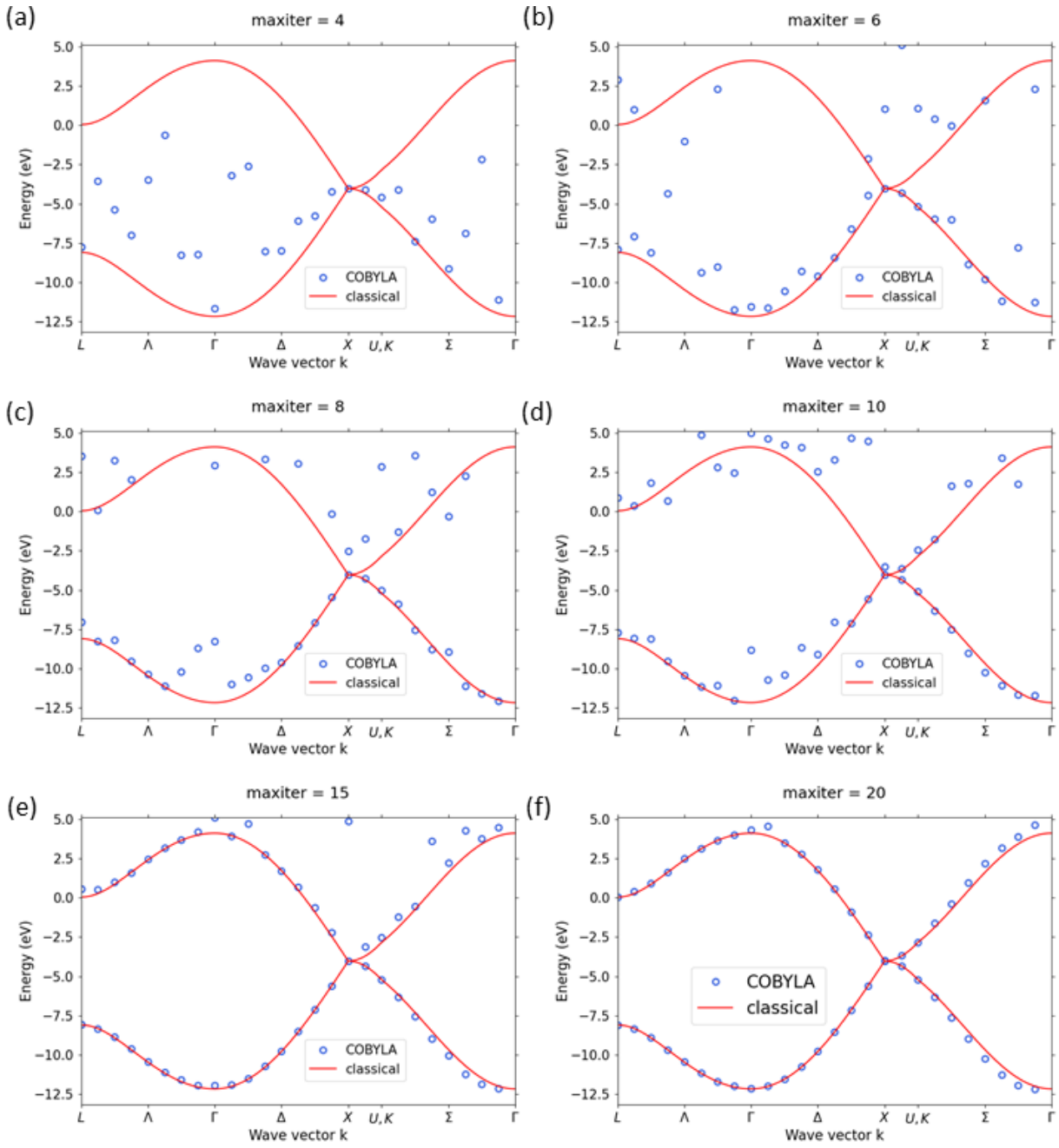

Figure 3 The computed energies of the two lowest bands within the band structure of Si as obtained by classical means (red curves) and from a simulator of the quantum processor (blue points) employing the COBYLA minimizer for a series of values of the maximum number of iterations (the MAXITER parameter).

After reporting results from simulations of the run of the quantum computer above, we next present a limited amount of results obtained employing the actual quantum computer (called “ibm_lagos”) within the IBM Quantum platform in **Figure 4**. Having the previous results from simulations of run of the quantum computer and experience related to a minimum number of iterations, we have set up the maximum number of iteration to a value which should guarantee reliable results, in particular, the MAXITER = 100. The obtained results for a few point along the lowest energy band, see the black circles in **Figure 4**, exhibit an excellent agreement with data calculated by classical means (red curves in **Figure 4**).

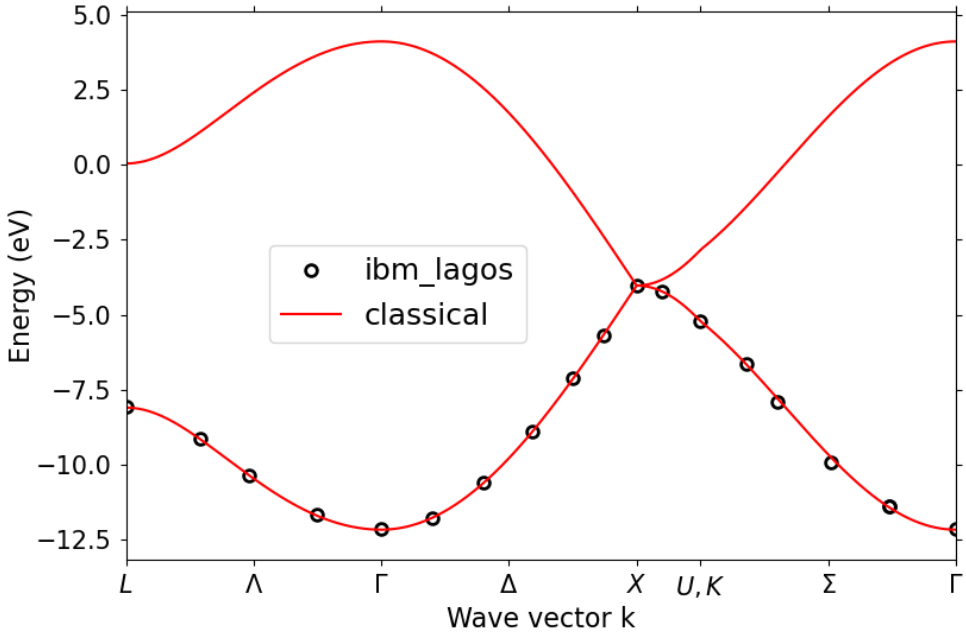

Figure 4 A few computed points from a real quantum processor called “ibm_lagos” as provided by the IBM Quantum platform. The results (black circles) are again compared with those obtained by classical means (red curves). The maximum number of iteration was set to MAXITER = 100.

4. CONCLUSION

We have performed a computational study of electronic band structure of crystalline diamond-structure silicon employing simulators of quantum computers as well as a real physical realization of a quantum processor. We focused on the lowest two occupied bands of Si and used a hybrid variational quantum eigensolver algorithm to compute the eigenvalues of a Hamiltonian set up within tight-binding type of crystal description. We thoroughly investigated sensitivity of the obtained results on computational parameters, in particular, the maximum number of iterations within the iterative optimization by the COBYLA optimization method. Employing first simulations of the run of quantum computer, we compared the results with values obtained by classical means.

We have found that (i) a few dozens of iterations are needed in order to obtain results with an acceptable accuracy and (ii) given a particular point in the reciprocal space, the state with a higher energy is computed reliably for a higher number of iterations than the state with a lower energy. Next, we have also obtained a few energies along the lowest energy band of the Si from several runs employing a physical realization of a quantum processor as provided by the IBM Quantum platform. Having the previous analysis of the sensitivity of the results from the simulator, we have set up the maximum number of iteration to a suitably high value and the quantum-computer energies showed an excellent agreement with those calculated by classical means.

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