Journal of Applied Physics REVIEW pubs.aip.org/aip/jap

Re-examination of important defect complexes in silicon: From microelectronics to quantum computing

Cite as: J. Appl. Phys. **137**, 230701 (2025); doi: 10.1063/5.0276550
Submitted: 18 April 2025 · Accepted: 2 June 2025 ·
Published Online: 17 June 2025

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ABSTRACT

The physical properties of silicon can be controlled by defects and impurities present in the lattice, with carbon, hydrogen, and oxygen being the most important impurities. During material processing, these impurities interact with each other leading to the formation of clusters. The T-center contains two inequivalent C atoms with one of the two linked to an H interstitial atom. The I-center contains at least one C, one H, and one O atom in its structure. The M-center contains at least two C atoms and an H atom, but its exact structure has not been definitely determined. The G-center contains a C substitutional and C interstitial pair, whereas the W-center is composed of three silicon self-interstitials. Here, we re-examine the structure and the electronic properties of carbon–hydrogen and carbon–hydrogen–oxygen defects (T, M, I, G, and W-centers) as these are presently important for emerging quantum technologies. We discuss experimental work and how recent theoretical calculations have furthered our knowledge of these important centers.

I. INTRODUCTION

Enhancing the output and functionality of semiconductor devices requires an in-depth understanding of the defect processes in semiconductor materials. Silicon (Si) has been the dominant material in microelectronics for decades, so there is an extended literature on the association of defects and impurities and their impact on physical properties and applications. Defect engineering is an important way to improve the potential of the material to be employed in applications from microelectronic to quantum technology.

The dominance of Si in the microelectronic era over competitive materials such as germanium (Ge) was mainly due to the advantageous material properties of its native oxide [i.e., silicon dioxide (SiO_2)]. The technological advancement of chemical vapor deposition (CVD) and molecular beam epitaxy (MBE) led to the sidelining of traditional methods such as thermal oxidation and paved the way for the introduction of high-k dielectric materials.[1–6] These gate dielectric materials diminished the importance of SiO_2, which was a key component of Si-based microelectronic devices. This led the research community and industry to reconsider alternative semiconductor materials such as Ge and silicon germanium ($Si_{1-x}Ge_x$), which possess better carrier mobilities, lower dopant activation energies, and smaller bandgap as compared to Si.[7–12]

Typically, impurities and intrinsic defects in Si (and Ge or $Si_{1-x}Ge_x$) can be introduced during single crystal growth via the Czochralski method, device processing, and in radiation environments.[13–17] Typical defects such as vacancy-oxygen pairs have been thoroughly investigated in Si (for example, Refs. 18–20

and references therein), there is regenerated interest for hydrogen-, carbon-, and oxygen-related defects. Although these impurities in Si, which are inadvertently added in the lattice during crystal growth or/and material processing, have been previously studied,[21–23] there is increased interest in the community. More specifically, the interactions among these impurities may lead to the formation of defect clusters that can have important applications in quantum technologies. It is also of interest that these defects can now be studied in a more rigorous theoretical way using advanced density functional theory techniques that were not available or were too computationally expensive a few years ago.

It was previously established that radiation damage or/and thermal treatments in Czochralski Si-containing hydrogen can produce a variety of secondary defects, which are well-known color centers with characteristic lines detected in the spectra received by luminescence spectroscopy. These are labeled: T (935.1 meV), I (965.2 meV), M (760.8 meV), G (969.5 meV), C (789.4 meV), W (1018.9 meV), X (1040.9 meV), and P (767.3 meV).[24] Color centers in semiconductors are impurities or defects some of which are potentially light-emitting structures in the lattice of semiconductors. In essence, these centers have the property to bind electrons to an extremely localized region, additionally exhibiting very exceptional spin and optical properties.[25–27] These centers have essentially regenerated the interest in Si now as a material for quantum technology applications (quantum computing, spin-to-phonon conversion, photonic memories, and integrated single-photon sources).[28–31] Indeed, such centers in Si as G, C, W, and T are prime candidates for spin-photon interfaces. The centers can trap single electrons and if these electrons were hit; for instance, with a laser, they emit photons in specific wavelengths. In other words, these centers possess levels in the Si bandgap, and the transition of electrons from these levels as a result of an external stimulus is accompanied by the emission of photons at certain frequencies. It has been found experimentally that they have a dominant zero-phonon line (ZPL) within the telecommunication bands, especially the O-band[32–34] in the range of 1260–1360 nm, allowing the transmission of a large amount of data with very high speed. To be useful for quantum communications, color centers should have ZPL transitions that split under a magnetic field and their ground states should have an unpaired electron spin (refer to Ref. 35 and references therein). In this category are the T, M, and I centers mentioned above,[35] the study of which is the main purpose of the present work. They are created by irradiation and subsequent thermal treatments (T, M, I) or/and only by thermal treatments (T, I).[36–40]

The aim of the present Review is to re-examine from an experimental and theoretical viewpoint important or potentially important defect centers in Si for quantum computing applications. We discuss in detail the elusive M-center and re-examine its potential structure. We investigate the defect centers studied experimentally for a number of years for their potential impact on microelectronic devices and their new application in the quest for qubits. We highlight the selection criteria for qubits and identify interesting systems to consider in Si. Finally, we discuss advances in theoretical calculations that could offer complementary information to experiment.

II. STRUCTURE OF CENTERS

A. The T-center

The T-center in Si emits a very technologically attractive wavelength of 1326 nm (935.1 meV) within the telecommunication O-band, providing compatibility with commercial low-loss components, and long-lived electron and nuclear spin memories. Optical centers are important in quantum optics, spintronics, quantum communications, sensing, and computing. The T-center with its narrow communication band, long spin coherence, and direct photonic integration is considered for use as a spin-photon interface for quantum computing and networking. From another point of view, Si that previously dominated microelectronics for nearly 60 years is now again at the forefront of technology due to the properties of color centers, as a material with the potential to improve quantum devices.[31–33] The T-center is a particularly promising defect due to its long spin lifetimes and spin-selective optical transitions.[35,41–48] Notably, despite being discovered long ago,[49,50] there is renewed interest in the T-center due to its potential as an emitting element. This provided the stimulus for detailed research that employed various experimental techniques mainly luminescence, infrared spectroscopy with the addition of isotope shifts and splitting of the relative lines, as well as electrical and magnetic measurements. The main purpose was to acquire the most complete knowledge of the properties and behavior of T-center and scrutinize its ability as an emitting defect structure for quantum technology applications.[41–62,55]

In the first work that reported[49] studies regarding T-center in samples containing different concentrations of C and O impurities, it was established that C is included in the structure of the defect, but oxygen is not. Irion *et al.*[50] confirmed the presence of C from the ^{13}C isotope shifts of the ZPL line of the center. In a similar way, the presence of H was verified[37] by studying the shift in the ZPL line in deuterium-diffused samples. In a subsequent study, Safonov *et al.*[59] determined a localized vibrational mode (LVM) splitting in four components in a ^{13}C silicon sample observed in PL. This implied that the T-center contains two inequivalent C atoms. Furthermore, the distinct shifts in the cases of H and D indicated that H is bonded with one of the two C atoms. The symmetry of the center is monoclinic I (C_{1h}).[35,59] The model suggested for the defect is a ⟨100⟩-oriented C–C pair occupying a substitutional site.[59–63] The H atom is attached to one of the carbon atoms, denoted as C_4, and the other undercoordinated atom is denoted as C_3. Figure 1 depicts the structure of the T-center.[59] The configuration of the defect is labeled[60] as $C_s(C_iH)_{\langle 100\rangle}$. Notably, the two C atoms are directly bonded sharing a substitutional site of a silicon atom. One of these C atoms is terminated with an H atom, leaving an unpaired electron dangling bond on the other C atom.[59] The formation of the defect occurs when a C_i atom traps an H atom in the BC-sited defect. This, in turn, diffuses in the lattice to be captured by a C_s atom, thus leading to a T-center. It was argued that this formation mechanism is more probable than that where an H atom is trapped by a dicarbon atom that is the C_i–C_s defect since the latter center is not stable[59,60] beyond ∼300 °C. However, in another theoretical study that involved an approximate molecular orbital method, it was found[64] that the second formation mechanism should also be considered. The C_i–C_s defect is metastable,

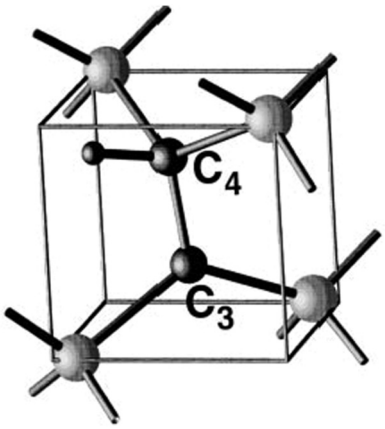

FIG. 1. A schematic representation of the T-center. Reproduced with permission from Safonov *et al.*, Phys. Rev. Lett. **77**, 4812–4815 (1996). Copyright 1996 American Physical Society.

having two configurations, labeled A and B. It was suggested[64] that the H atom could be attached to a bond of one of the C atoms of the C_i–C_s defect in the B-form configuration. The T-center is responsible for an acceptor level (−/0) located in the upper half of the gap at E_c-0.27 eV.[59–63]

It should be noted that in samples with large H concentrations, it was determined that the amplitude of the T-line in the PL spectra was significantly lower. This was explained by considering that the initially formed C_i–H defect instead of combining with a C_s to form T-center may trap a second H atom becoming immobile and thus preventing the formation of the T-center. An alternative possibility is that in samples with such high hydrogen concentrations, T-centers themselves may rapidly trap a second H atom leading to the formation of a C_2H_2 complex. Three possible configurations were investigated[60] with the most stable being the $(C_2H_2)_{\langle 100\rangle}$ structure (refer to Fig. 2).

B. The I-center

The I-center possesses a luminescence line at 965.2 meV within the telecommunication band; however, it has not been studied as extensively as the T-center. It is produced[36,65–67] either by radiation damage of Cz–Si followed by annealing at about 450 °C or/and by simple thermal treatment at temperatures above 450 °C, similar to the T-center. Isotope shift measurements[63,64,68] of the ZPL with H and D confirmed the presence of H, while a study with ^{12}C and ^{14}C confirmed the presence of C. Furthermore, the study of the shifts of the local modes has shown[65,66] that the I-center contains two inequivalent C atoms in its structure. Regarding the presence of oxygen in the defect, the first indirect evidence is that the center is the dominant luminescence line in Cz–Si, but it is not observed in Fz–Si.[36] Additionally, Si doped with an isotope mixture of ^{16}O–^{18}O proved unequivocally that at least one oxygen atom is present.[66] A close parallel has been drawn between I- and T-centers since the ZPL energies are similar, and

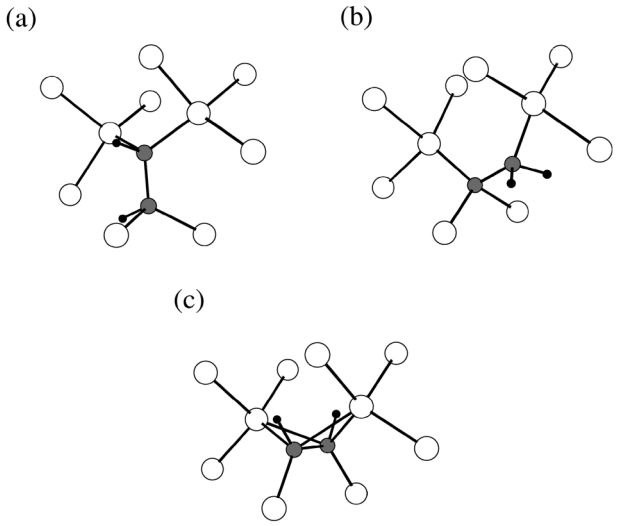

FIG. 2. Schematic of the three possible structures of the C_2H_2 split-interstitial defect: (a) The $(C_2H_2)_{\langle 100\rangle}$, (b) the $(C_2H_2)_{BC}$, and (c) the $(C_2H_2)_{\langle 110\rangle}$ configuration. Reproduced with permission from Leary *et al.*, Phys. Rev. B **57**, 3887–3899 (1998). Copyright 1998 American Physical Society.

the effect of stress and magnetic fields is also similar.[50,62] The two centers have C_{1h} symmetry as uniaxial stress measurements indicated, and both have a primary axis close to ⟨001⟩.[68] The similarity of the electronic structure and the local modes of the I and T-centers suggests that the I-center is simply a T-center structure perturbed by a nearby oxygen atom.[62,68] Since the two lines of I- and T-centers are close (they occur at 935.2 and 935.1 meV, respectively), one expects that their corresponding levels in the Si gap should be also close. The I-center has an acceptor level (−/0) at a higher energy position than that of T-line. The suggested positions of the levels[59,61] are E_c-0.17 eV for the I-center and E_c-0.2 eV for the T-center. Although the exact position of the oxygen atom in the I-center structure is not definitely known, it was suggested[69] that the oxygen atom is placed in either the Si–Si bonds adjoining to the C_3 atom preserving the C_{1h} symmetry.

C. The M-center

The M-center, with a photoluminescence line at 760.8 meV within the telecommunication band, has not been investigated so extensively and intensively as the T-center. The M-line was reported more than 50 years ago[70] in electron-irradiated silicon after annealing at 350 °C. Initially, it was found that the M-center contains C, and it was considered[50] as a parent defect of the T-center. In a later work, it was shown that it also contains hydrogen.[37] The main difference between the two lines is that the T-line appears also in heat-treated Si without any radiation damage although the M-line appears in the PL spectra only after irradiation and subsequent annealing.[38,71–73] Importantly, another difference between T- and M-centers in the case of irradiated samples is that the M center appears after annealing at a lower temperature

(350 °C) than the T-center (450 °C).[71] This is consistent with the suggestion[50] that the M-center is a parent defect for the T-center but may be inconsistent for the case of the formation of T-center only through thermal treatment without previous irradiation since in the latter case the M-center is not formed. The T-center is also formed with an alternative mechanism that does not presuppose the previous formation of the M-center, that is, through the formation reaction[64] $C_i + H_i \rightarrow (C_i–H_i)$, $(C_i–H_i) + C_s \rightarrow (C–C–H)$.

Additional detailed studies[74] of the M-center have confirmed, from the analysis of isotope splitting, the presence of one hydrogen atom and at least two carbon atoms in the M-center. There is no evidence[74] that the center contains oxygen. Regarding its atomic structure, the results suggested that the M-center,[74] and more specifically, the configuration of the two carbon atoms in the defect structure, has similarity with that of the $C_i–C_s$, well known as the G photoluminescence center. The M-line has a triclinic C_1 symmetry and creates an acceptor level at E_c-0.37 eV.[74,75] Furthermore, the study[74] of the local modes of the M and G lines suggests that both centers contain a carbon atom at the same location within their structures. As the M-center (conversely to the T-center) is produced only in irradiated Si after annealing at temperatures above 300 °C, and the $C_i–C_s$ disappears from the spectra in the temperature range[76] of about 250–330 °C the following formation mechanism for the M-center could be envisaged: $C_i–C_s + H \rightarrow (C–C–H)$. This mechanism is based on the evidence that the $C_i–C_s$ center does not break up when the center is annealing out, but rather it is converted to another configuration where it becomes mobile and captures a hydrogen atom.[71–74] The suggested reaction mechanism is consistent with the experimental evidence that the M-center is formed only after irradiation and subsequent thermal anneals since it presupposes the existence of the G-center that needs irradiation to be formed. We notice that a third C-type configuration of the $C_i–C_s$ has been reported, which is more stable than the A- and B-types mentioned above.[64,77] In this configuration, the C–C atom pair along the ⟨100⟩ direction occupied a regular lattice site in the Si lattice. This arrangement has been considered[64] as an alternative configuration of the T-center (refer to Fig. 5b in Ref. 64). However, the latter configuration suits also well with the experimental data so far available for the M-center as referred to above, and we tentatively suggest Fig. 5b in Ref. 64 as a potential candidate for the latter center. Of course, additional results of both experimental and theoretical studies are required to further verify such an assignment.

D. The G-center

The C_iC_s defect is known as the G-center and is a very important radiation-induced defect in Czochralski-grown Si. It has been identified in the IR spectra by an LVM at 607 cm^{-1}.[78] The introduction of the optically active G-centers is an approach for improved efficiency due to the sharp luminescence peak at 1.28 μm, which matches the optical communication wavelength of 1.30 μm, and it has been shown that G-centers contribute to optically pumped lasing.[79–81] The bistability of the G-center is key for its emission properties.[79–81] In particular, Song *et al.*[82] determined that there are two configurations of the G-center using experimental techniques. Theoretical calculations can provide complementary information to experiment and subsequently determine a third plausible configuration for C_iC_s.[83–86] Figures 3(e)–3(g) summarize the DFT results by Wang *et al.*[86] and the three configurations of C_iC_s.

Song *et al.*[82] established the bistable A- and B-type interstitial-carbon–substitutional-carbon pair in Si. Thirty-five years ago, however, the $C–C_iC_s$ was predicted using DFT calculations in more recent studies.[84–86] The potential structures for the Si tri-interstitial as derived by DFT are reported in Fig. 4.

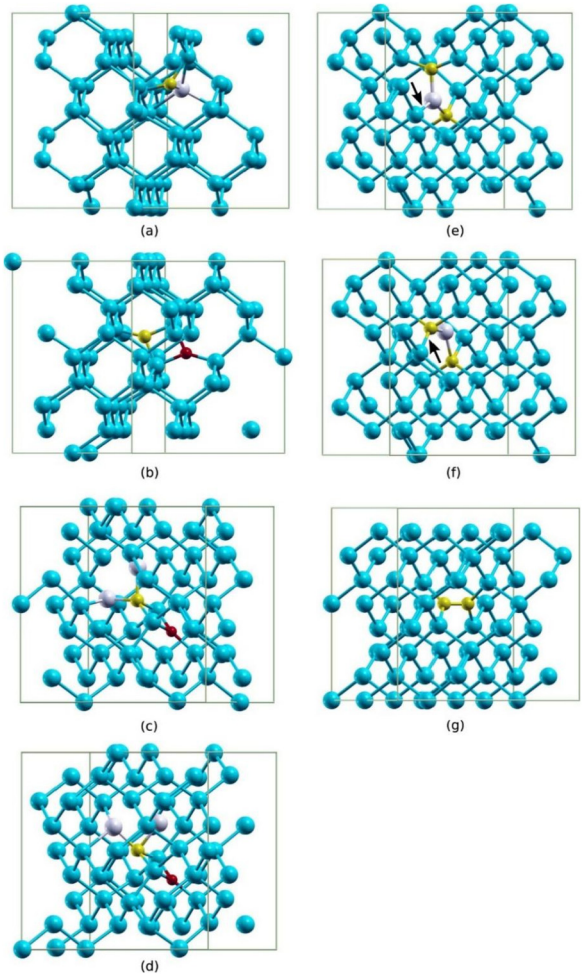

FIG. 3. Schematic representations of (a) C_i (Si_I), (b) C_iO_i, (c) $C_iO_i(Si_I)_a$, (d) $C_iO_i(Si_I)_b$, (e) A-type C_iC_s, (f) B-type C_iC_s, and (g) C-type C_iC_s. The blue spheres represent the Si atoms, red spheres represent the O atoms, and yellow spheres represent the C atoms. With gray, the following Si atoms are marked: (i) The Si_I atom in C_i (Si_I), (ii) the Si atom in-between two C atoms in A-C_iC_s and B-C_iC_s, and (iii) the two Si atoms exhibiting a substantial position change between the $C_iO_i(Si_I)$ structures. Arrows denote the breaking and forming of bonds during the transition between A-C_iC_s and B-C_iC_s. From Wang *et al.*, Sci. Rep. **4**, 4909 (2014). Copyright 2014 Author(s), licensed under a Creative Commons Attribution (CC BY) license.

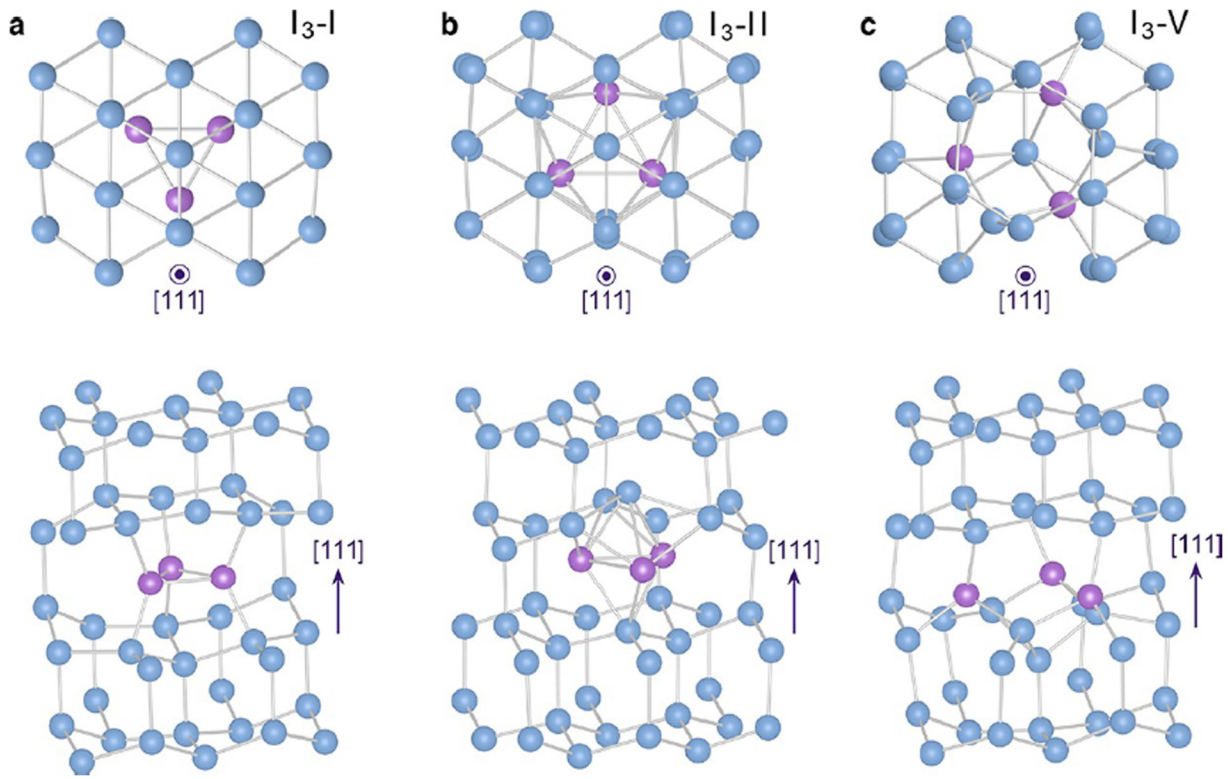

FIG. 4. Possible structures for the Si tri-interstitial as derived by DFT derived. These are possible configurations of the W-center in Si. Reprinted with permission from Baron *et al.*, ACS Photonics **9**, 2337–2345 (2022). Copyright 2022 American Chemical Society.

E. The W-center

Si self-interstitial defects and clusters have been investigated for years.[27,87–89] The W-center is a self-interstitial complex containing three silicon interstitial atoms, and its emission is assigned to the phonon-free luminescence line at 1218 nm (1.018 eV).[90,91] The W-center in Si was initially considered by the community as self-interstitials in Si can degrade the performance of microelectronic devices.[92] They can be formed during radiation, laser annealing, and implantation; however, their exact structure is somewhat controversial.[93–95]

III. QUANTUM EMITTERS IN SI

Quantum technologies will have a profound impact on productivity and revolutionize scientific discovery (i.e., discovery of novel materials) and many technological sectors including energy, communications, sensing, and health. The building elements of quantum computing are quantum bits (qubits) and can be derived from different ways (i.e., for example, trapped ions, photons, spin, and charge state in quantum dots).[96] This is of particular interest as qubits are the spin-dependent point defects in semiconductor materials that essentially form a two-level system.[97,98] Forming qubits for quantum circuits has led researchers to consider a number of materials including, gallium arsenide,[99] diamond,[100,101] germanium,[102,103] and silicon.[104–107]

The key advantage of Si is that there is very significant know-how on its crystal growth, device fabrication, and material properties for over 60 years. Key advantage for Si is the relative ease of integration in electronics and photonics, scalability, and bright photon emission in the telecommunication band.[48,51,108,109] If the most important emitters in Si were selected, these would be the G-, W-, and T-centers.[51] These contain common elements (i.e., C and/or H) or intrinsic defects (i.e., Si_I). Under equilibrium conditions and considering diffusion issues, these common components in the centers will not form adequate concentrations of the centers required for technological application. To form localized and optimized centers processing with thermal annealing, ion implantation, and local excitation (i.e., ion beams and laser pulses) is required.[110–113] In Si devices, laser processing is used for localized annealing, and as such, it is implemented in defect engineering.[114]

IV. PERSPECTIVES

A. Challenges and materials and systems to consider

To systematically understand the design criteria for a physical system to be appropriate for use as qubits, Weber *et al.*[115] devised a set of rules that describe the ideal host. Specifically, they mentioned

that a wide bandgap structure is required to avoid unnecessary thermal excitations with bound states that are separated from each other in the bandgap. Furthermore, the defects should exhibit a paramagnetic ground state capable of encoding the quantum information and also have a small spin–orbit coupling to avoid unwanted spin-flips. Nowadays, there are many variations in these rules as it was extremely difficult to find the ideal structure, and so the smaller bandgap semiconductors, such as Si, are studied as potential qubit hosts. In addition to using point defects as qubits, as it is used in Kane's quantum computer,[116] near-infrared (NIR) color centers have also been explored for quantum optics applications. In this subsection, we examine the characteristics, performance, and prospects of the recently studied defects in Si as well as alternative systems that could be worth exploring.

Bergeron *et al.*[35] were among the first to investigate the T-center defect in Si and its emission in the telecommunications O-band as a promising candidate for spin-photon interfaces and quantum technologies. In their work, they used isotopically purified ^{28}Si, and they demonstrated that the T-center possesses both long-lived spin coherence and efficient optical transitions that are crucial for qubits.[35] Furthermore, the experiments showed a paramagnetic ground state while one of the excited states contained a singlet. The first complete theoretical work of the potential of T-center for qubit applications was done by Dhaliah *et al.*[42] where they first presented a complete study of the excitation processes for the T-center. The authors used advanced computational methods such as hybrid functionals within the classical and constraint DFT framework, and they reveal that the first excited state is created from a defect bound-exciton, where an electron occupying the delocalized valence band edge is excited to the highly localized gap state. To our knowledge, this was the first time that a qubit protocol is proposed, and it does not involve excitation within two gap states; however, attention should be paid to bound-electron excitations as it is often that the valence band edge electron cannot be excited to a localized state due to symmetry selection rules, as, for example, in silicon vacancy center in diamond.[117,118] The authors reported a long radiation lifetime of 5 μs for the spin allowed transition, which was consistent with the experimental reports, while it was also longer than the N*V* center in diamond. As they report, the neutral charge state is favorable for all Fermi levels across the bandgap, and the ZPL was calculated at 0.985 eV, in good agreement with the experimental value. However, as they report in their work, while T-center is charge stable, it is highly sensitive to hydrogenation, which can occur under annealing conditions. This requires careful experimental fabrication as well as controllable environmental conditions of operation as it is possible to destroy the quantum information or even the magnetic properties if the purity of the defect is damaged. Furthermore, while there are very extensive studies on the T-center or similar defects and their potential is undeniable, attention should be paid to the effect of the spin–orbit coupling effect and strength, as it is possible that a high SOC strength can introduce unwanted intersystem crossings as Weber *et al.*[115] described in their work.

Baron *et al.*[95] reported using experiments and theory the first optical detection and characterization of W-centers in Si and revealed its potential to quantum technologies. He used photoluminescence measurements at low temperatures and found single photon emitters at 1.218 μm, which belongs to the telecom O-band, and the excited state lifetime was approximately 30 ns. The electronic structure of this defect is reported in the same work, and the authors concluded that the transition is again in the form of a bound exciton, involving, however, a transition from an occupied gap level below the valence band and above the conduction band. Similar to the T-center, while these transitions provide appropriate ground states and excitation energies, their main disadvantage is the low temperature they require for operation. The low temperature is required to avoid thermal excitations that can manipulate the quantum information. The G-center in Si is also an experimentally well-studied defect that has recently gained attention for quantum applications although its electronic structure was revealed very recently by Udvarhelyi *et al.*[119] This structure when in the neutral charge state has a singlet ground state with an optically active singlet excited state with a ZPL at 0.97 eV. As it is reported, there is a meta-stable triplet state between the two singlets, which shows the observed detected magnetic resonance, as well as the zero-field splitting and hyperfine tensors reported experimentally.[120,121] This defect is one of the few cases where the quantum information is not encoded in a paramagnetic ground state, but instead in the paramagnetic excited state and while there are some notable studies of defects, they remain relatively rare and less explored.

In their work, Xiong *et al.*[57] performed high-throughput research for the identification of promising quantum defects for quantum information technologies. For this work, more than 1000 charged defects were investigated by combining semilocal DFT with a recently developed method called "single-shot" hybrid functional method (HSE0). While many prior research papers focus on the excitation between two discrete defect levels of the bandgap, this study considered optical excitations similar to T-center. Furthermore, they used as selection criteria the spin multiplicity of the ground state, the strength of the dipole moment, and the ZPL value. Within this framework, they identified titanium (Ti_i^+), iron (Fe_i^0), and ruthenium (Ru_i^0) interstitials as strong candidates for emission to the telecommunication wavelength. It was observed (refer to Fig. 3 of Ref. 57) that the transitions are from occupied defect levels in the gap to the conduction band minimum for Ti_i and Fe_i, while for Ru_i, the excitation is to the defect levels that appear in the conduction band.

From all the above, the movement around Si for quantum technologies are undeniable with a number of defects being in the spotlight as potential candidates. The investigation of T-center and related defects (although providing the desirable optical and magnetic properties) requires low-temperature operation to avoid unnecessary excitations, and this is a significant disadvantage. However, due to the compatibility with the current CMOS circuit architecture, it is highly likely that these defects will serve as the first step for quantum architectures, but eventually different systems should be examined that offer room-temperature operation. Erbium (Er) impurities in Si have also attracted attention, and according to our opinion they serve as a compelling alternative platform for quantum technologies due to its ability to emit to the telecom band, which is ideal for long-distance fiber optic-based communications.[122,123] The Er ion is a rare-earth impurity with f-orbitals and undergoes intra-4f shell transitions that are protected

from the host lattice. This results in sharp optical lines and long coherence times even at room temperatures. This makes Er^{3+} a strong candidate for integrating single photon emitters that are compatible with current electronics.

B. Advances in theoretical methods

For a number of years, the quest for ideal quantum defects was plagued by expensive computations and inaccurate results especially using classical functionals such as Perdew–Burke–Ernzerhof (PBE) and local density approximation (LDA) functionals. These inaccuracies are not only the underestimation of bandgap, which is well reported but also inaccurate stable charges,[124] and it is logical to assume that this will result in inaccurate charge transition levels and formation energies. For this reason, it is crucial to use more advanced levels of theory such as hybrid DFT functionals but at high computational cost. Recently, Abbas *et al.*[125] presented a comprehensive study of SCAN and r^2 SCAN meta-GGA functionals for modelling N*V*-center-like defects in SiC. The authors compare these functionals against PBE and HSE06, and they found that meta-GGA offers significant improvements over PBE in key properties for quantum technologies, such as radiation lifetime and ZPL. The findings underscore that meta-GGA have also the potential for large-scale high-throughput investigations.

V. CONCLUSIONS

In the present Review, we considered typical defects in silicon and in particular T-, M-, I-, G-, and W-centers. These defects have been investigated by the community for decades due to their impact on microelectronic devices, but now there is renewed interest due to their potential application in quantum computing. We highlight the selection criteria for qubits and identify interesting legacy and novel systems to consider in Si. The latter include Er, Fe, Ru, and Fe defects in Si. Finally, we discuss meta-GGA approaches that offer a computationally economical (as compared to hybrid DFT) and precise way to generate complementary information to experiment.

AUTHOR DECLARATIONS

Conflict of Interest

The authors have no conflicts to disclose.

Author Contributions

P. P. Filippatos: Conceptualization (equal); Writing – original draft (equal); Writing – review & editing (equal). **A. Chroneos:** Conceptualization (equal); Writing – original draft (equal); Writing – review & editing (equal). **C. A. Londos:** Conceptualization (equal); Writing – original draft (equal); Writing – review & editing (equal).

DATA AVAILABILITY

Data sharing is not applicable to this article as no new data were created or analyzed in this study.

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