Ernst, O. C., D. Uebel, and J. Acker. 2026. Isotopic Engineering of Silane: Scaling quantum grade 28SiH4 Synthesis for the Next Generation of Semiconductor Technologies. In *Silicon for the chemical and solar industry XVIII*, edited by M. Tangstad, H. Rong, A. Valderhaug, B. Andresen, H. Dalaker, and I. G. Page. Kristiansand, Norway, September 7–10, 2026. https://doi.org/10.55669/oa900805

Isotopic Engineering of Silane: Scaling quantum grade $^{28}SiH_4$ Synthesis for the Next Generation of Semiconductor Technologies

O. C. Ernst, D. Uebel, and J. Acker
Brandenburg University of Technology Cottbus-Senftenberg, Germany, owen.ernst@b-tu.de

Keywords: Isotopic Engineering, Silicon-28, Monosilane Synthesis, Quantum Technology, SiF_4 Conversion

Abstract –This work addresses a critical chemical bottleneck in quantum hardware scaling by demonstrating a high-purity, high-yield conversion from isotopically enriched silicon fluoride precursors to electronic-grade monosilane-28. An analytical framework for the synthesis and chemical vapor deposition (CVD)-validation of the isotopes are imperative to bridge the gap between specialized nuclear enrichment and global semiconductor fabrication, essential for the realization and scalability of fault-tolerant quantum computing.

While the chemical purification of natural silicon to electronic grade (9-11N) is a mature industrial process, the emerging field of 2nd generation quantum technologies impose new restrictions: the elimination of nuclear noise. Natural silicon contains ~4.7% of the stable isotope ^{29}Si, whose nuclear spin acts as a decoherence source for charge carrier spin states used as qubits. To enable fault-tolerant quantum computing, an industrial value chain for chemically and isotopically pure "quantum grade" ^{28}Si is required. Despite projections indicating that demand already surpasses 100 million USD annually, a scalable value chain for this critical material has yet to be developed.

This work revisits a pathway for the production and analytical evaluation of high quality ^{28}Si. Isotopic enrichment is achieved via gas counter current centrifugation of silicon tetrafluoride. The subsequent transformation into viable monosilane is a critical prerequisite for further processing. This is achieved using highly potent hydrogenation processes. Gas-Mass Spectrometry (G-MS) verify chemical quality of 4 N after chemical purification. The main contaminants are traced back to carbon residues from chemical conversion.

To validate the materials performance in a semiconductor environment, purified monosilane was used for the epitaxial growth of Si thin films via CVD. Secondary Ion Mass Spectrometry (SIMS) confirm the preservation of isotopic purity >99.9% throughout the deposition process and provide high-sensitivity depth profile of carbon contaminants.

1. INTRODUCTION

Isotopically engineered materials possess altered chemical and physical properties, rendering them attractive for various technical applications. One notable example of increasing relevance is the silicon-28 isotope (^{28}Si) and its precursor gas monosilane-28 ($^{28}SiH_4$).

^{28}Si is of crucial importance as a material platform for both spin-based quantum computing and spintronics (Ernst et al., 2022; Kane, 1998; Liu et al., 2022). The quality of the material platform is defined by its isotopic purity, as nuclear spins of odd-numbered isotopes such as ^{29}Si interact with the charge carrier spins via Fermi contact interaction and significantly reduce their decoherence time. Conversely, even-numbered isotopes, such as ^{28}Si, are characterized by a lack of nuclear spin ($\bar{I}$ =0 ħ). This is referred to in the literature as a "spin vacuum."

Reducing the ^{29}Si content from 4.7 % to 1 ppm has been shown to result in an augmentation of the decoherence time from T_2=20 µs to T_2=60 s (Witzel et al., 2010).
Two-dimensional electron gases (2DEG) and hole gases (2DHG) at the interface of ^{28}Si heterostructures are used to isolate, manipulate and measure charge carrier spins, and ultimately use them as quantum bits (qubits – basic unit of information in a quantum computer). Electron spin qubits on 300-mm Si-wafers already exhibit high fidelity values of >99% (two-qubit control fidelity and measurement fidelity), thereby demonstrating the principle scalability of the approach (Steinacker et al., 2025). However, the coherence of the systems is currently limited to T_2^{echo}≈100–800 ms (Scappucci et al., 2021; Witzel et al., 2010; Zwerver et al., 2022). The underlying reason is the present low material quality of isotopically pure ^{28}Si, which is required for the production of the qubits. In this paper, "isotopically pure ^{28}Si" refers to silicon whose isotopic ^{28}Si content has been increased from 92.2 mol-% to at least 99.9 mol-%.

Furthermore, ^{28}Si possesses the highest thermal conductivity ever measured for a dielectric. At 450 W/cm·K at 21 K, this value exceeds the conductivity of natural silicon (^{nat}Si) by a factor of 10 (Inyushkin et al., 2018, 2004). This renders the semiconductor attractive for low-temperature physics and microelectronic components with high heat generation.

Further applications are derived from the bandgap that is shifted by 58 meV (Karaiskaj et al., 2001). High-energy measurements have been shown to provide a more precise fine structure of the non-phononic photoluminescence lines of bound excitons, which result, for example, from B-doping. The optimized fine structure in the photoluminescence spectrum can be used for high-resolution studies of exciton processes in isotopically pure materials, for example in quantum sensing.

The value chain for ^{28}Si is characterized by its complexity and high cost. It necessitates the implementation of elaborate enrichment and chemical conversion processes, resulting in a distinctive chemical fingerprint. The resulting impurities reduce the coherence time of the charge carriers (Itoh and Watanabe, 2014; Witzel et al., 2010): The T_2^{echo} time decreases from 60 s to 200 ms at donor concentrations C_E=1.2×10^{14} /cm^3 with 1 ppm ^{29}Si.

Until 2022, material was globally procured from Russia through individual R&D channels. Political realities following Russia's invasion of Ukraine, characterized by geopolitical tensions and the imposition of trade restrictions, lead to a critical supply and material shortage. For industrial manufacturers, these issues present a technical and economic challenge, stemming from limited availability and inadequate material quality. The shortage lead to elevated prices, regularly exceeding 100 EUR/g for silicon-28-tetrafluoride ($^{28}SiF_4$), and 1'000 EUR/g for $^{28}SiH_4$ and ^{28}Si (Ernst et al., 2026). Its current research demand already supersedes 15 million EUR annually in Europe with the outlook to grow to 100 million EUR annually until 2030. Projections indicate that the global demand already surpasses 100 million USD annually, which corresponds to an annual volume of 100 kg.

A critical bottleneck in the value chain concerns the chemical transformation from industrially available silicon-28-tetrafluoride ($^{28}SiF_4$) to $^{28}SiH_4$ and other chemical vapor deposition (CVD) precursor materials, since this is the only step not covered by a commercial institution. Reliable instrumental methods for cost-effective purification and ensuring the chemical and isotopic purity of ultra-pure gases are still missing.

The limited availability of ^{28}Si has recently been classified as a "key vulnerability" by the Transatlantic Quantum Community (TQC) in 2025. The report *Critical Vulnerabilities in the*

Quantum Computing Supply Chain within the NATO Alliance (2025) recommends "[to] develop an understanding of the key requirements needed to support the fabrication of semiconductor spin systems, including any specialized requirements for the successful integration of isotopically pure ^{28}Si into the process flow."
In this paper, we provide a concise overview of the complex value chain for isotopically pure semiconductors and the synthesis methods for $^{28}SiH_4$ methods that have been employed to date. Laboratory-synthesized $^{28}SiH_4$ is analyzed for its chemical and isotopic purity and deposited as ^{28}Si layers using a rudimentary thermal CVD setup. Secondary ion mass spectrometry (SIMS) measurements of the layer provide a quantitative basis for demonstrating its chemical quality. The chemical quality of the layer exceeds the chemical quality of Russian samples reported in the literature and is sufficiently high to produce quantum bits from it.

2. MAJOR SECTION

2.1 Value chain

2.1.1 Isotopic separation

A multitude of physical methods have been developed for the purpose of isotopic enrichment (Ernst et al., 2024). However, from an economic standpoint, the use of counter-current gas centrifuges has proven to be the most viable option to date.

In gas centrifuges, isotopic enrichment is achieved by exploiting the mass-dependent inertia of molecules. Isotope separation is achieved using rotating cylinders. A gas introduced into the cylinders is subjected to continuous acceleration. The resulting inertial force, denoted by F, can be calculated using the simple equation

$$F = M v^2 r^{-1} \quad [1]$$

(with M – molar mass; v – rotational velocity; r – radius of the cylinder)

and ensures isotope separation.

Enrichment of ^{28}Si is typically carried out using SiF_4, as it is among the limited number of Si compounds that meets the critical chemical and physical requirements (Borisevich and Levin, 2001; Levin, 1994):

i. The vapor pressure of the substance in question must exceed 5–10 mmHg (≙ 0.7–1.3 kPa), as enrichment requires a stable gaseous source.

ii. The substance must not undergo chemical reactions with the materials of the enrichment chamber, which are typically stainless steel or specialized high-temperature alloys.

iii. For sufficient enrichment, the molecular mass of the molecules must not be less than 40 u. SiH_4, with a molecular mass of 32 u, is therefore not suitable. It has been demonstrated that higher molecular masses generally result in higher enrichment rates and lower energy consumption.

iv. The substance to be enriched must exhibit sufficiently high thermal stability.

v. No chemical reaction should occur between the molecules of the substance intended to be enriched. Anion exchange or atom exchange would result in incomplete enrichment.

Modern gas centrifuges, also known as ZIPPE or KAMENEV centrifuges, consist of vertically rotating cylinders typically made of carbon fiber-reinforced steel with a cylinder radius of 5 cm and reaching rotational speeds of 750 m/s and higher (Kushner, 2013). High rotational speeds are achieved by a rotating magnetic field that sets the cylinder itself in rotation. A force of up to 12,000 eVm (>1,000,000 g) acts on each SiF_4 molecule. This force is counteracted by a pressure gradient between the gas compressed against the cylinder wall and the vacuum generated at the axis of rotation. If the pressure at the wall is excessively high due to elevated circulation speeds, the gas may condense on the walls of the centrifuge.

In the counter-current centrifuge, in addition to the gas flow from the inside to the outside, a vertical pressure difference arises that pushes the molecules near the axis of rotation downward (or upward). By heating the cylinder head and altering the geometry of the cylinder's interior, a counter current can be generated that maintains or even amplifies the internal pressure differences. The flow generates horizontal zones within the cylinder. In each zone, horizontal enrichment occurs from the inside (light molecules) to the outside (heavy molecules). Due to the vertical pressure difference, the heavy molecules are gradually transferred to the zone above (or below), while the light molecules migrate to the zone on the opposite side. The degree of enrichment increases with each additional zone.

Two strategies were pursued in the past. On the one hand, many short centrifuges can be connected. The degree of enrichment can be increased by connecting the centrifuges in series, and throughput can be increased by connecting them in parallel. This technical solution is highly adaptable and allows for swift adjustments to system parameters or product requirements. The second strategy on the other hand is based on a small number of tall centrifuges. These enable the generation of multiple enrichment zones within a single cylinder. As a result, the process is accelerated and requires fewer maintenance-intensive individual components. Additionally, contamination from cylinder walls and gas lines is minimized. A challenge associated with this method pertains the stability of the tall cylinders. When the rotary motors start up, the bending frequencies of the cylinders must be overcome. Cylinders longer than 1 m are susceptible to critical deformation if they are not stabilized.

Urenco Ltd. is the world's largest producer of isotopically pure materials and relies exclusively on counter-current gas centrifuges. Only the enrichment plants of the Russian TVEL Fuel Company, a subsidiary of the state-owned Atomenergoprom Group, possess a comparable production capacity. Both Urenco and TVEL have demonstrated that they can achieve enrichment levels of $^{28}SiF_4$ up to 99.9999%.

Alternative isotope separation methods include gas thermodiffusion, laser separation, cyclotrons, and air nozzle processes (Ernst et al., 2026, 2024).

2.1.2 Chemical conversion

$^{28}SiF_4$ is not generally considered suitable for the majority of industrial CVD processes. One reason for this is the molecule's exceptionally high negative standard formation enthalpy (<-1500 kJ/mol (Sukkaew et al., 2016)). The Si-F bond is regarded as the strongest single bond ever measured. A variety of other silane species, including monosilane SiH_4 and trichlorosilane $HSiCl_3$, are employed in industrial settings as CVD precursors.

The transformation of inert fluorides into isotopically pure semiconductor precursors poses a particular challenge (Figure 1). The chemical reduction of $^{28}SiF_4$ has been the subject of scientific inquiry since the 1960s as a method for producing $^{28}SiH_4$.

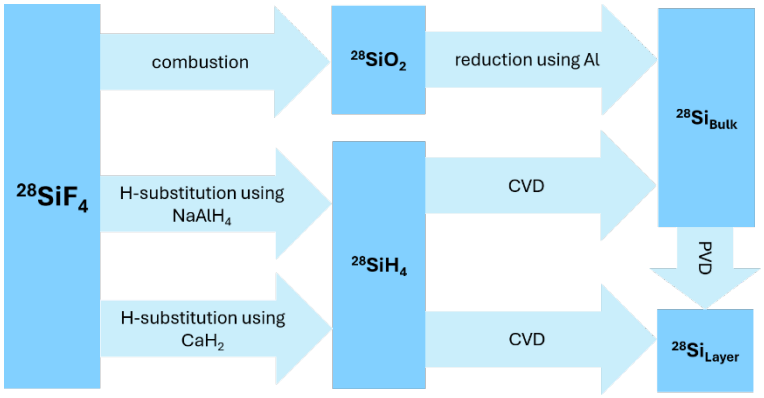

Figure 1: Strategies for the synthesis of $^{28}SiH_4$ and ^{28}Si starting from $^{28}SiF_4$.

In general, the quantitative conversion of semimetal halides (MXy) into their hydrogen compounds (MHy) is possible using hydrides (AHx).

$$MX_y + AH_x \rightarrow MH_y + AX_x \quad [2]$$

In the literature, conversions were executed using dissolved alkali hydrides containing aluminum (Al), lithium (Li), sodium (Na), or combinations thereof. However, the necessary dissolution of these hydrides in organic solvents such as dimethyl ether, diethylene glycol, or tetrahydrofuran result in indelible C-impurities (Devyatykh et al., 2003; Sennikov et al., 2015).

Alternatively, solid calcium hydride (CaH_2) can be brought into reaction with $^{28}SiF_4$ directly, thereby circumventing the introduction of critical impurities (Bulanov et al., 2008, 2004, 2002).

$$2\ CaH_2 + {}^{28}SiF_4 \rightarrow 2\ CaF_2 + {}^{28}SiH_4 \quad [3]$$

However, this conversion method is hindered by the high $^{28}SiF_4$ pressures necessary to attain sufficient reaction velocity and consequently the necessity for extensive safety measures.

2.2 Chemical and isotopic purity from literature

The enrichment of $^{28}SiF_4$ is feasible on an industrial scale, and the material is available on the global market for less than 500 EUR/g from companies such as Urenco Ltd. or Orano S.A.. The challenge lies in the chemical conversion of the fluoride to $^{28}SiH_4$ and ^{28}Si (Ernst et al., 2024).

Initial experiments were conducted in the United States in 1958 (Gordon and Bowers, 1958). The primary strategy entailed the conversion of $^{28}SiF_4$ to $^{28}SiO_2$, followed by reduction with aluminum powder at a temperature of 1100 °C.

$$^{28}SiF_4 + O_2 \rightarrow {}^{28}SiO_2 + 2\ F_2 \quad [4]$$

$$3\ {}^{28}SiO2 + 4\ Al \rightarrow 3\ {}^{28}Si + 2\ Al_2O_3 \quad [5]$$

The method was revived in 1994 in an American-Russian-German study. $^{28}SiO_2$ was sourced from the Oak Ridge National Laboratory (ORNL) and the Russian National Metrology Institute (NMI) (Becker et al., 2010, 2009). It is noteworthy that the NMI material was discarded due to high levels of impurities of unknown origin, while the ORNL material was reduced using the Al method described above in a collaboration between the Physikalisch-Technische Bundesanstalt (PTB) and Wacker-Chemitronic in Germany. The resulting ^{28}Si crystals, with a mass of 300 g, exhibited high impurity levels of C (1.3×10^{17} cm^{-3} / 2.6 ppm), O (1.1×10^{16} cm^{-3} / 0.22 ppm), and B (10^{18} cm^{-3} / 20 ppm).

In experiments conducted in the 1980s and 1990s, reduction was carried out using lithium aluminum hydride ($LiAlH_4$) and sodium aluminum hydride ($NaAlH_4$) (Ulmer et al., 1982). However, the resulting fluoride salts cause the solvent to become sludgy, making the implementation and scaling of these processes technically very difficult. Furthermore, the solvent introduces organic solvents that can act as carbon sources—electrically active donors in silicon. Furthermore, metals present in silicon exhibit electrical activity, necessitating sophisticated and expensive purification process. However, yields of over 99% have been reported (Sennikov et al., 2015, 2010).

Progress was achieved using the approach in which solid CaH_2 was used for reduction. Given the high cost of $^{28}SiF_4$, efficiency plays a pivotal role. For the CaH_2 approach, efficiencies of up to 90% have been reported (Bulanov et al., 2004; Sennikov et al., 2015, 2010).

Table I: A selection of isotopically pure silicon compounds from the literature, alongside a comparison of their purities with those in this study. Chemical impurities are measured either in SiH_4 gas (ppm) or in solid Si (cm^{-3}). However, these measurements cannot be directly compared.

	reference	compound	producer	method of synthesis	isotopic purity	chemical impurities
1	(Sennikov et al., 2010)	$^{28}SiH_4$	Russian Federal State Institution of Science Institute of Chemistry of High-Purity Substances (IChHPS)	CaH_2 / cryo-filtration/ ultra-purification	99.9 %	< 1ppm
2	this work	$^{28}SiH_4$	Brandenburg Technical University (BTU)	$LiAlH_4$	>99.9 %	0.12 % H_2O 200 ppm CO_2 80 ppm CH_4 < 10 ppm other
3	(Becker et al., 2010)	^{28}Si	ORNL / Wacker-Chemitronic	$^{28}SiO_2$-reduction	99.99 %	1.3×10^{17} cm^{-3} C 1.1×10^{16} cm^{-3} O 10^{18} cm^{-3} B
4	(Becker et al., 2009)	^{28}Si	IChHPS / Leibniz Institute of Crystal Growth (IKZ)	CaH_2 / CVD /Float zone	99.9999 %	< 10^{15} cm^{-3}
5	(Liu et al., 2022)	^{28}Si	IChHPS / Leibniz Institute of Crystal Growth (IKZ)	CaH_2 / CVD / Float zone	99.9 %	10^{18} – 10^{20} cm^{-3} C
6	this work	^{28}Si	BTU / [qgm]	$LiAlH_4$ /CVD	>99.9 %	10^{17} – 10^{19} cm^{-3} C

It has been observed that both the $NaAlH_4$ process as well as the CaH_2 process are affected by SiF_4 residues and CO_2 and CH_4 impurities (Sennikov et al., 2010). Due to their high vapor pressures, these impurities remain even during cryogenic distillation. In order to achieve the required level of chemical purity, a series of purification steps, collectively referred to as "ultrapurification", were implemented. These steps included cryofiltration and the separation of light and heavy fractions. These processes, in turn, result in a lower overall yield.

2.3 Experimental results and discussion

2.3.1 Synthesis and characterization of as-synthesized $^{28}SiH_4$

To replicate and verify literature values, $^{28}SiH_4$ was synthesized from $^{28}SiF_4$ in a laboratory-scale setup using $LiAlH_4$. The synthetic route closely follows previously published protocols (Ernst et al., 2025, 2026; Ulmer et al., 1982). To archive this, gaseous $^{28}SiF_4$ was sparged through a solution of $LiAlH_4$ in anhydrous tetrahydrofuran (THF) under an inert atmosphere. Efficient gas-liquid mixing can be ensured by utilizing a fine-pored glass frit or a Venturi system. Due to the exothermic nature of the reaction, continuous colling was applied to maintain the internal temperature strictly below the boiling point of THF (66°C). The detailed chemical procedure can be adopted from these references. The gas quality was analyzed using a GSD 320 Omnistar gas mass spectrometer (Pfeiffer Vacuum GmbH.).

The initial gas mass spectrometry analysis of the as-synthesized gas confirmed the successful formation of $^{28}SiH_4$. As illustrated in Figure 2, the mass spectrum exhibits prominent peaks at m/z=15,16,18,28,29,30,31,32,42,44,62,85. Quantitative evaluation of the impurity profile reveal that the as-synthesized gas contains significant volatile contaminants, predominantly tetrahydrofuran THF (9,4 %), methane (1,9 %), water (0,42 %), and carbon dioxide (0,39 %). THF is used as solvent for the $LiAlH_4$-agent and remains at the vapor phase after the primary reaction stage. Likewise, the methane likely originates from the solvent. The origin of the significant levels of water and carbon dioxide is not clear but may be attributed to minor atmospheric leaks within the experimental setup and residues inside the setup. While no distinct signals for molecular oxygen or nitrogen were resolved, trace amounts may be masked by the dominant $^{28}SiH_x^+$ fragmentation (m/z = 28–32) or rapidly consumed via reaction with $^{28}SiH_4$ prior to reaching the detector of the mass spectrometer.

The conversion of $^{28}SiF_4$ to $^{28}SiH_4$ is almost complete. It has been determined that only 0.35 mol% of $^{28}SiF_4$ is detectable in the as-synthesized gas. This corresponds to a chemical yield of approximately 99.6%. As a potential byproduct of the reaction, traces of disilane Si_2H_6 (21 ppm) were detected.

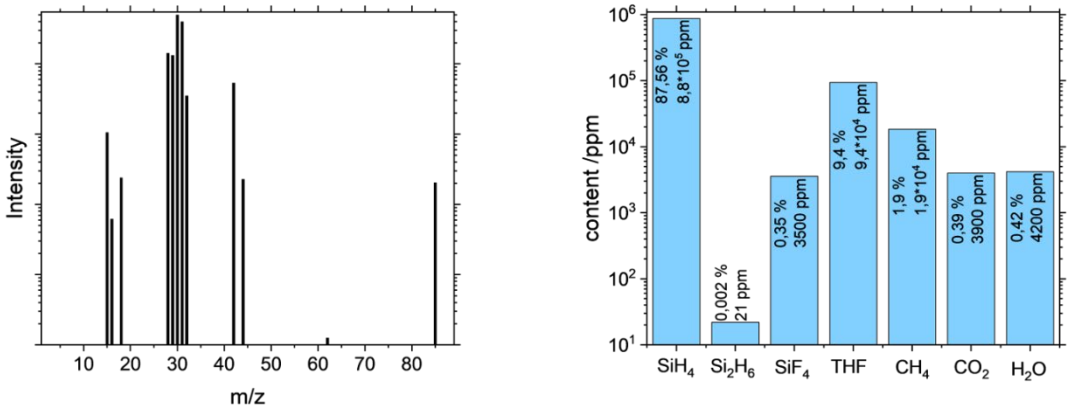

Figure 2: Results of the gas mass spectrometry analysis of the as-synthesized SiH_4. The contaminants likely originate from the $LiAlH_4$ solvent, unreacted SiF_4, and minor gas leaks.

2.3.2 Purification of $^{28}SiH_4$

To meet the stringent purity requirements for subsequent CVD deposition, the as-synthesized gas was subjected to cryogenic distillation at a temperature of 180 K. Since the boiling point of SiH_4 lies at 168 K, it is expected that all high-boiling impurities will be frozen out.

The post-purification mass spectrum (Figure 3) demonstrates a substantial reduction in all volatile impurities, shifting the baseline closer to or even below the detection limit. Specifically, THF, SiF_4 and Si_2H_6 content dropped below the detection limit of 10 ppm. Even though the boiling point of methane is lower than 180 K, the methane concentration also dropped by more than two orders of magnitude to 80 ppm. It is likely that a significant portion of the methane is redissolve in the frozen THF.

The concentrations of water (0.12%) and carbon dioxide (200 ppm) remain high. This supports the hypothesis that this contamination is caused by small leaks in the laboratory setup or residue on the setup wall.

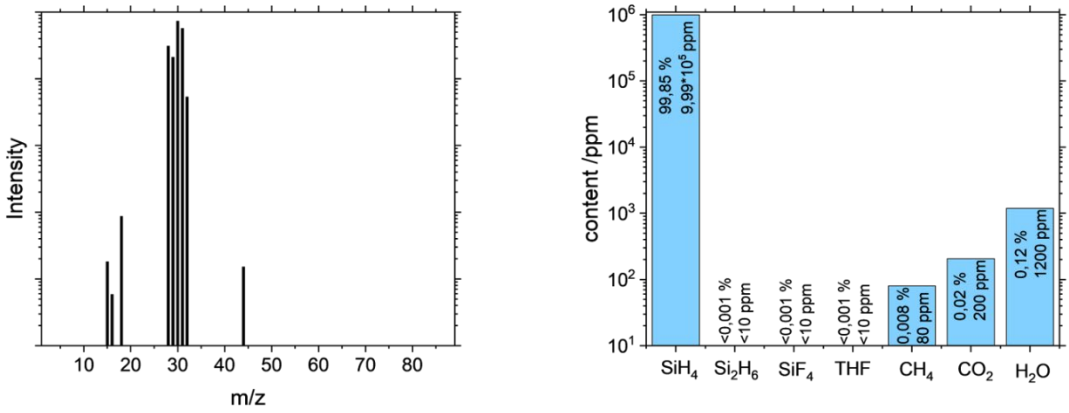

Figure 3: Results of the gas mass spectrometry analysis of the purified SiH_4. Purification was performed at 168 K.

2.3.3 Thin-film deposition and Secondary Ion Mass Spectrometry

As gas-phase mass spectrometry is primarily sensitive to chemical impurities rather than isotopic variations and the detection limits are rather high, the purified $^{28}SiH_4$ was subsequently deposited as a solid thin film.

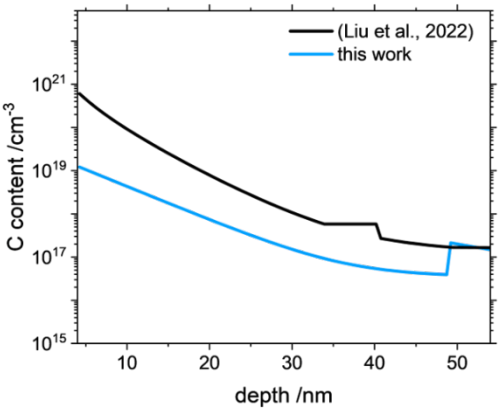

Figure 4: Results of the SIMS analysis for Carbon Content of Si layers deposited from the purified SiH_4 in comparison with previous results.

A CVD process was conducted within a quartz tube furnace at 650°C for a duration of 10 min. The substrates used in this study were HF-dipped 1×1 cm^2 Si(100) wafers. The resulting Si-layers exhibit a thickness of approx. 50 nm and were subjected to analysis by Secondary Ion Mass Spectrometry (SIMS) utilizing a Cameca ims 4f-E6 (Cs^+, 14.5 eV, SI^-) to analyze the critical C impurities.

As illustrated in Figure 4, the layers exhibit a C content ranging from 10^{17} cm^{-3} to 10^{18} cm^{-3} (5 ppm to 50 ppm). These impurities are attributed to CH_4, which deposits heavily alongside SiH_4. In a previous study (Liu et al., 2022), we obtained purified $^{28}SiH_4$ from the Russian IChHPS and deposited the material. In the initial 50 nm of the layer, a C content ranging from 10^{19} cm^{-3} to 10^{20} cm^{-3} (0,05 % to 0,5 %) was measured. Therefore, we cannot confirm the very low carbon content of the Russian material (<1 ppm) reported in the literature for the sample we received.

The isotopic content was also measured (Figure 5). It has been demonstrated that the isotopic purity of the source $^{28}SiH_4$, respectively $^{28}SiF_4$, can be transferred to the ^{28}Si layers. The isotopic distribution in natural silicon is as follows: 92.3% ^{28}Si, 4.7% ^{29}Si, and 3.0% ^{30}Si. In the $^{28}SiF_4$ employed as the source material, the ^{28}Si content was enriched to 99.9%. The isotopic composition of the deposited ^{28}Si sample was found to be approximately 0.01% ^{29}Si and 0.001% ^{30}Si, which corresponds to the purity in the $^{28}SiF_4$ source. Thus, it has been demonstrated that the chemical conversion of $^{28}SiF_4$ to $^{28}SiH_4$, followed by CVD deposition as ^{28}Si, does not result in the introduction of measurable isotopic impurities. Therefore, the process preserves isotopic purity.

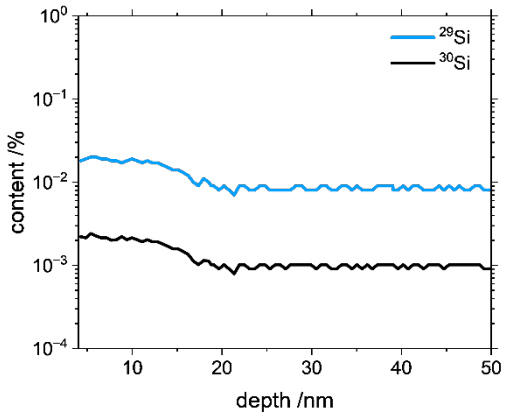

Figure 5: Results of the isotopic SIMS analysis of deposited Si layers from (Liu et al., 2022).

3. CONCLUSIONS

^{28}Si is a critical raw material that will become increasingly important as second-generation quantum technologies approach maturity. However, to date, no Western company has succeeded in establishing commercial-scale production of ^{28}Si or $^{28}SiH_4$ to supply the market with the 100 kg per year currently needed. Despite the existence of established processes for the enrichment of $^{28}SiF_4$, the subsequent conversion to $^{28}SiH_4$—and particularly its purification—remains challenging.

In this study, we have shown that $^{28}SiH_4$ can be synthesized using $LiAlH_4$ utilizing the synthesis protocols from literature. However, the C impurities introduced by the necessary

solvent, particularly CH_4, cannot be removed without multi-step cryofiltration and fractionation. This observation is consistent with reports in the literature.

A comparison of our material with Russian-produced material, manufactured using the CaH_2 process, shows that our material has a carbon content that is 1.5 to 2 orders of magnitude lower. However, the literature frequently describes lower carbon content measurements, which were generally preceded by additional solid-phase purification via Float Zone.

In this study, we also demonstrated that the isotopic purity of $^{28}SiF_4$ can be transferred to both $^{28}SiH_4$ and, in the subsequent CVD step, to ^{28}Si layers.

Based on these results, the $LiAlH_4$ route has the potential to yield high-quality $^{28}SiH_4$. However, in order to render the material suitable for utilisation within the semiconductor industry, reliable purification methods must be employed that, in contrast to established methods, do not result in a significant reduction in the overall process yield.

4. ACKNOWLEDGEMENTS

This work was funded by the EXIST research transfer project 03EFBB0063 HoCHQuant, supported by the German Federal Ministry for Economic Affairs and Energy and the ESF.

5. REFERENCES

Becker, P., Friedrich, H., Fujii, K., Giardini, W., Mana, G., Picard, A., Pohl, H.-J., Riemann, H., Valkiers, S., 2009. The Avogadro constant determination via enriched silicon-28. Meas. Sci. Technol. 20, 092002. https://doi.org/10.1088/0957-0233/20/9/092002

Becker, P., Pohl, H. -J., Riemann, H., Abrosimov, N., 2010. Enrichment of silicon for a better kilogram. physica status solidi (a) 207, 49–66. https://doi.org/10.1002/pssa.200925148

Borisevich, V.D., Levin, E. V., 2001. SEPARATION OF MULTICOMPONENT ISOTOPE MIXTURES BY GAS CENTRIFUGE. Sep. Sci. Technol. 36, 1697–1735. https://doi.org/10.1081/SS-100104759

Bulanov, A.D., Balabanov, V. V., Pryakhin, D.A., Troshin, O.Yu., 2002. Preparation and Fine Purification of SiF4 and 28SiH4. Inorganic Materials 38, 283–287. https://doi.org/10.1023/A:1014735203351

Bulanov, A.D., Mikheev, V.S., Troshin, O.Yu., Lashkov, A.Yu., 2008. Reaction of silicon tetrafluoride with calcium hydride as a propagating wave. Russian Journal of Inorganic Chemistry 53, 6–10. https://doi.org/10.1134/S0036023608010026

Bulanov, A.D., Moiseev, A.N., Troshin, O.Yu., Balabanov, V. V., Isaev, D. V., 2004. Fine Purification of Monoisotopic Silanes 28SiH4 , 29SiH4 , and 30SiH4 via Distillation. Inorganic Materials 40, 555–557. https://doi.org/10.1023/B:INMA.0000031984.83652.87

Devyatykh, G.G., Dianov, E.M., Bulanov, A.D., Troshin, O.Yu., Balabanov, V. V., Pryakhin, D.A., 2003. Preparation of High-Purity Monoisotopic Silane: 28SiH4, 29SiH4, and 30SiH4. Doklady Chemistry 391, 204–205. https://doi.org/10.1023/A:1025380518197

Ernst, O., Uebel, D., Boeck, T., 2025. EP000004486690A1: METHOD FOR PRODUCING ISOTOPE-ENRICHED GERMANIUM-HYDROGEN COMPOUNDS.

Ernst, O.C., Liu, Y., Boeck, T., 2022. Leveraging dewetting models rather than nucleation models: current crystallographic challenges in interfacial and nanomaterials research. Zeitschrift für Kristallographie-Crystalline Materials 237, 191–200.

Ernst, O.C., Uebel, D., Brendler, R., Handschick-Ernst, A., Acker, J., 2026. Halbleiter für Quantumcomptuting: Wertschöpfung und chemischer Fingerabdruck. AMA Service GmbH, Von-Münchhausen-Str. 49, 31515 Wunstorf, Germany, pp. 80–83. https://doi.org/10.5162/iCCC2026/4.6

Ernst, O.C., Uebel, D., Brendler, R., Kraushaar, K., Steudel, M., Acker, J., Kroke, E., 2024. Silicon-28-Tetrafluoride as an Educt of Isotope-Engineered Silicon Compounds and Bulk Materials for Quantum Systems. Molecules 29, 4222.

Gordon, J.P., Bowers, K.D., 1958. Microwave Spin Echoes from Donor Electrons in Silicon. Phys. Rev. Lett. 1, 368–370. https://doi.org/10.1103/PhysRevLett.1.368

Inyushkin, A. V, Taldenkov, A.N., Ager III, J.W., Haller, E.E., Riemann, H., Abrosimov, N. V, Pohl, H.-J., Becker, P., 2018. Ultrahigh thermal conductivity of isotopically enriched silicon. J. Appl. Phys. 123, 095112. https://doi.org/10.1063/1.5017778

Inyushkin, A. V, Taldenkov, A.N., Gibin, A.M., Gusev, A. V, Pohl, H.-J., 2004. On the isotope effect in thermal conductivity of silicon. physica status solidi (c) 1, 2995–2998. https://doi.org/https://doi.org/10.1002/pssc.200405341
Itoh, K.M., Watanabe, H., 2014. Isotope engineering of silicon and diamond for quantum computing and sensing applications. MRS Commun. 4, 143–157. https://doi.org/10.1557/mrc.2014.32
Kane, B.E., 1998. A silicon-based nuclear spin quantum computer. Nature 393, 133–137. https://doi.org/10.1038/30156
Karaiskaj, D., Thewalt, M.L.W., Ruf, T., Cardona, M., Pohl, H.-J., Deviatych, G.G., Sennikov, P.G., Riemann, H., 2001. Photoluminescence of Isotopically Purified Silicon: How Sharp are Bound Exciton Transitions? Phys. Rev. Lett. 86, 6010–6013. https://doi.org/10.1103/PhysRevLett.86.6010
Kushner, D., 2013. The real story of stuxnet. IEEE Spectr. 50, 48–53. https://doi.org/10.1109/MSPEC.2013.6471059
Levin, E. V., 1994. Separation of multicomponent isotopic mixtures in a gas centrifuge — approximate method for solving the system of diffusion-transport equations and analysis of some separation characteristics. Atomic Energy 77, 760–767. https://doi.org/10.1007/BF02415435
Liu, Y., Rinner, S., Remmele, T., Ernst, O., Reiserer, A., Boeck, T., 2022. 28Silicon-on-insulator for optically interfaced quantum emitters. J. Cryst. Growth 593, 126733. https://doi.org/https://doi.org/10.1016/j.jcrysgro.2022.126733
Scappucci, G., Taylor, P.J., Williams, J.R., Ginley, T., Law, S., 2021. Crystalline materials for quantum computing: Semiconductor heterostructures and topological insulators exemplars. MRS Bull. 46, 596–606. https://doi.org/10.1557/s43577-021-00147-8
Sennikov, P.G., Kornev, R.A., Abrosimov, N. V., 2015. Production of stable silicon and germanium isotopes via their enriched volatile compounds. J. Radioanal. Nucl. Chem. 306, 21–30. https://doi.org/10.1007/s10967-015-4192-4
Sennikov, P.G., Kotkov, A.P., Adamchik, S.A., Grishnova, N.D., Chuprov, L.A., Ignatov, S.A., 2010. Impurities in monosilanes synthesized by different processes. Inorganic Materials 46, 358–363. https://doi.org/10.1134/S0020168510040072
Steinacker, P., Dumoulin Stuyck, N., Lim, W.H., Tanttu, T., Feng, M., Serrano, S., Nickl, A., Candido, M., Cifuentes, J.D., Vahapoglu, E., Bartee, S.K., Hudson, F.E., Chan, K.W., Kubicek, S., Jussot, J., Canvel, Y., Beyne, S., Shimura, Y., Loo, R., Godfrin, C., Raes, B., Baudot, S., Wan, D., Laucht, A., Yang, C.H., Saraiva, A., Escott, C.C., De Greve, K., Dzurak, A.S., 2025. Industry-compatible silicon spin-qubit unit cells exceeding 99% fidelity. Nature 646, 81–87. https://doi.org/10.1038/s41586-025-09531-9
Sukkaew, P., Ojamäe, L., Kordina, O., Janzén, E., Danielsson, Ö., 2016. Thermochemical Properties of Halides and Halohydrides of Silicon and Carbon. ECS Journal of Solid State Science and Technology 5, P27–P35. https://doi.org/10.1149/2.0081602jss
Ulmer, H.E., Pickens, D., Rahl, F.J., Lefrancois, P.A., 1982. Producing silane from silicon tetrafluoride . US4407783A.
Witzel, W.M., Carroll, M.S., Morello, A., Cywiński, Ł., Sarma, S. Das, 2010. Electron spin decoherence in isotope-enriched silicon. Phys. Rev. Lett. 105, 187602.
Zwerver, A.M.J., Krähenmann, T., Watson, T.F., Lampert, L., George, H.C., Pillarisetty, R., Bojarski, S.A., Amin, P., Amitonov, S. V, Boter, J.M., Caudillo, R., Correas-Serrano, D., Dehollain, J.P., Droulers, G., Henry, E.M., Kotlyar, R., Lodari, M., Lüthi, F., Michalak, D.J., Mueller, B.K., Neyens, S., Roberts, J., Samkharadze, N., Zheng, G., Zietz, O.K., Scappucci, G., Veldhorst, M., Vandersypen, L.M.K., Clarke, J.S., 2022. Qubits made by advanced semiconductor manufacturing. Nat. Electron. 5, 184–190. https://doi.org/10.1038/s41928-022-00727-9

Dr. Owen C. Ernst
Research project lead, Brandenburg University of Technology Cottbus-Senftenberg
CEO, quantum grade materials [qgm] GmbH

Owen C. Ernst holds degrees in chemistry and physical chemistry from Humboldt University in Berlin, Germany. He led the “Local Growth and Structure Formation of Semiconductors” research group at the Leibniz Institute for Crystal Growth. Since 2024, he serves as the research project lead for "Chemistry and Physics of Isotopically Engineered Semiconductors" at Brandenburg University of Technology Cottbus-Senftenberg. In 2026, he founded the university spin-off quantum grade materials [qgm] GmbH.