January 14, 2026

Mitsubishi Electric Corporation

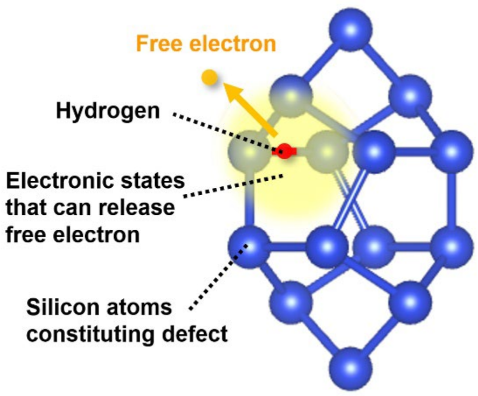
Institute of Science Tokyo

University of Tsukuba

Quemix Corporation

Mechanism of Hydrogen-driven Free-electron Generation in Silicon Elucidated for First Time Ever

Will enhance electron-concentration control in silicon power semiconductors to reduce power losses



Mechanism by which hydrogen generates free electrons via an interaction with the defect in silicon

Mitsubishi Electric Corporation, Institute of Science Tokyo, University of Tsukuba, and Quemix Corporation announced today that they have achieved the world's first[1] elucidation of how hydrogen produces free electrons[2] through the interaction with certain defects[3] in silicon. The achievement has the potential to improve how insulated gate bipolar transistors (IGBTs) are designed and manufactured, making them more efficient and reducing their power loss. It is also expected to open up possibilities for future devices using ultra-wide bandgap (UWBG) materials.[4]

In the global drive toward carbon neutrality, efforts to make power electronics more efficient and energy-saving are accelerating worldwide. IGBTs are key components responsible for power conversion, so improving their efficiency is a major priority. While hydrogen ion implantation has been used for about half a century to control electron concentration in silicon, the underlying mechanism has remained unclear until now.

In 2023, Mitsubishi Electric and University of Tsukuba jointly discovered a defect complex[5] in silicon that contributes to increasing electron concentration. They confirmed that this complex is formed when an interstitial silicon pair and hydrogen bind, but the reason why free electrons are newly generated in this process

1 According to research conducted by Mitsubishi Electric as of January 14, 2026.

2 Electrons that can move freely within a silicon crystal. Their concentration is controlled by the intentional introduction of specific Impurities.

3 Structural imperfections that affect the mobility and recombination of free electrons.

4 Diamond, aluminum nitride, etc. semiconductors with a larger bandgap than conventional silicon or silicon carbide semiconductors.

5 A defect complex composed of intrinsic defects—such as silicon interstitials—and extrinsic defects, like hydrogen. In power semiconductors, such defect complexes are intentionally created to control device performance.

was still unclear.[6] By using advanced computational calculations, the four organizations have now uncovered how hydrogen exists inside the defect complex. They have also explained why hydrogen releases electrons and how these electrons become free within silicon. Furthermore, their findings suggest that this mechanism could also be applied to diamond, a promising material for future power semiconductors that is difficult to control in terms of electron levels.

The full details of this research were published online on January 13 (London time) in *Communications Materials*, a journal published by Nature Portfolio.

Features

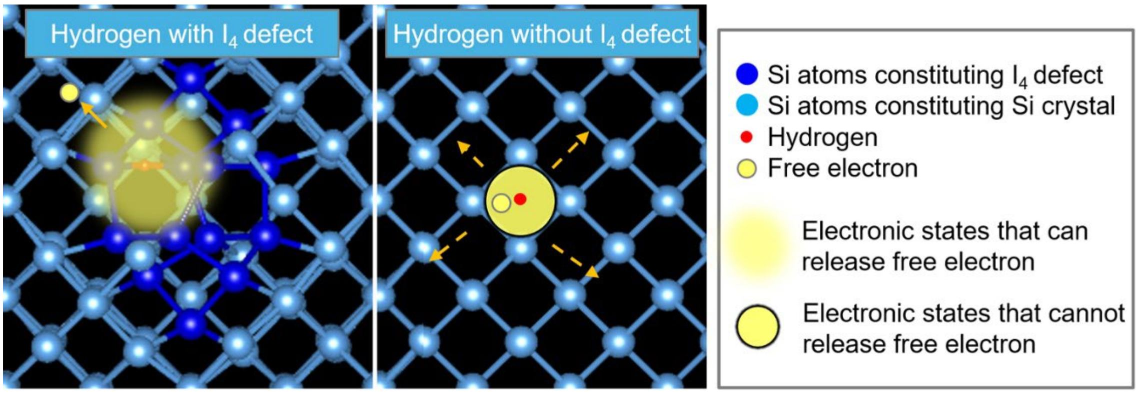
1) Mechanism by which a hydrogen-containing defect complex in silicon generates free electrons

For nearly half a century, hydrogen ion implantation into silicon was reported to produce free electrons at locations where hydrogen atoms are present. This technique is now used to form *n*-type layers containing free electrons inside power semiconductors such as IGBTs. However, an isolated hydrogen atom in silicon does not necessarily release a free electron,[7] so the underlying mechanism remained unclear.

Starting from the hypothesis that hydrogen and crystal defects act together to generate free electrons, joint research by Mitsubishi Electric and University of Tsukuba applied electrical and optical measurements and electron spin resonance (ESR).[8] In 2023, this work identified the I_4 defect—a structural disturbance formed by extra silicon atoms inserted into the silicon crystal—as being involved in free-electron generation. To clarify hydrogen's role, Institute of Science Tokyo and Quemix performed first-principles calculations[9] to models containing hydrogen atoms at multiple candidate sites around the I_4 defect to study the resultant structural stability and electronic states[10] of defect complexes.

The calculations showed that in defect-free silicon, a hydrogen atom forms electronic states that do not contribute to free-electron generation. However, when an I_4 defect is nearby, a hydrogen atom can reside in the center positions of bonds[11] between silicon atoms. In that configuration, the electronic states associated with the I_4 defect shift into a condition that favors electron release. In further analysis based on molecular orbital theory,[12] the computational calculation indicates a cooperative effect: an electron associated with a hydrogen atom moves to the I_4 defect, and the I_4 defect then releases an electron that functions as a free electron. This synergy between defect and hydrogen explains the observed free-electron generation.

6 "How does hydrogen transform into shallow donors in silicon?", *Phys. Rev.* B 108, 235201 (2023).
7 In a defect-free silicon, hydrogen atoms settle into positions known as *tetrahedral sites or bond-centered sites*, depending on their charge states where they form an electronic state that cannot generate free electrons.
8 A spectroscopy technique used to detect unpaired electrons in a magnetic field.
9 A computational method that predicts the material properties based on the laws of quantum mechanics, without relying on experimental data.
10 The energy level of an electronic state is important to control electron concentration, because if thermal energy exceeds this level, electrons can be thermally excited and become available as free electrons.
11 Bonds within a crystal are the forces that make atoms or molecules keep specific crystal structure, influencing the material's physical properties such as hardness, electrical conductivity and melting point.
12 A theory used to understand the arrangement and energy states of electrons within a molecule.



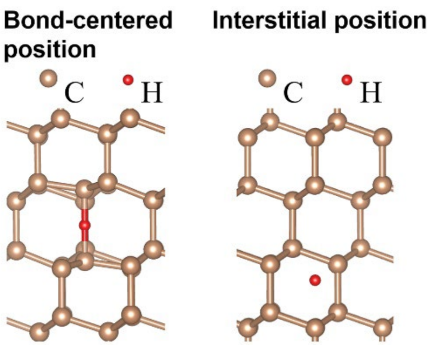
Schematic of free electron generation from hydrogen via the synergetic interaction with the defect

2) Technical demonstration: Up to 20% reduction in power loss in silicon IGBTs and diodes

Mitsubishi Electric has been reducing power loss in silicon IGBTs and diodes by combining hydrogen ion implantation for *n*-type layer formation and reducing the thickness of silicon substrates. For example, in a 1,200V-class device, the company has technically demonstrated reductions in total power loss of 10% in IGBTs and 20% in diodes compared with its 7th-generation products. The fundamental insights gained on hydrogen-related free-electron generation, which contributed to the present mechanism elucidation, have supported these power-loss reductions.

3) Theoretical indication of applicability to UWBG materials

Materials such as diamond and aluminum nitride (AlN) are promising for use in future power semiconductors and quantum sensors, but practical implementation has been hampered by the extreme difficulty of controlling electron concentration via conventional methods. To examine whether the hydrogen-related free-electron generation mechanism found in silicon could operate in UWBG materials, initial first-principles calculations were performed. The results indicate that in diamond—which shares a covalent crystal structure similar to silicon—hydrogen is energetically more stable when incorporated into bonds between carbon atoms rather than occupying interstitial gaps. When paired defects are present, this bond-center incorporation of hydrogen could enable the same kind of mechanism to function in diamond. This finding suggests a possible route to address electron-concentration control in certain UWBG materials, at least from a fundamental perspective.



Structural configuration of a hydrogen atom within a diamond crystal

Roles

Organization	Responsibilities
Mitsubishi Electric	1. Evaluation using electrical and optical measurements 2. Identification of the defect contributing to electron concentration 3. Construction of mechanism models
Institute of Science Tokyo	1. First-principles calculations based on the density functional theory (DFT)[13] 2. Elucidation of interactions between hydrogen and defects 3. Construction of mechanism models
University of Tsukuba	1. Evaluation using ESR technique 2. Identification of the defect contributing to electron concentration 3. Construction of mechanism models
Quemix	1. First-principles calculations based on the DFT 2. Elucidation of interactions between hydrogen and defects 3. Construction of mechanism models

This work was supported by Japan Society for the Promotion of Science (JSPS) KAKENHI under Grant-Aid for Scientific Research (nos. 21H04553,20H00340, and 22H01517). Additional support was provided by Center of Innovation for Sustainable Quantum AI (JST, grant number JPMJPF2221).

Future Development

By applying this mechanism to UWBG materials such as diamond, in which electron concentration traditionally has been difficult to control, this approach is aimed at advancing the development of semiconductor devices. These include power semiconductors, high-frequency devices and quantum sensors, all of which are expected to contribute significantly toward the achievement of a carbon-neutral world.

Publication

Title	Advancing N-type doping in semiconductors through hydrogen-defect interactions
Authors	Akira Kiyoi, Yusuke Nishiya, Yuichiro Matsushita & Takahide Umeda
Journal	Communications Materials (a journal published by Nature Portfolio)
Date	January 13, 2026 (London time)
DOI	10.1038/s43246-025-00955-4

[13] A quantum mechanics-based computational method that treats electron density as a fundamental variable and calculates electronic states to predict the properties of materials.

###

About Mitsubishi Electric Corporation

With more than 100 years of experience in providing reliable, high-quality products, Mitsubishi Electric Corporation (TOKYO: 6503) is a recognized world leader in the manufacture, marketing and sales of electrical and electronic equipment used in information processing and communications, space development and satellite communications, consumer electronics, industrial technology, energy, transportation and building equipment. Mitsubishi Electric enriches society with technology in the spirit of its "Changes for the Better." The company recorded a revenue of 5,521.7 billion yen (U.S.$ 36.8 billion*) in the fiscal year ended March 31, 2025. For more information, please visit www.MitsubishiElectric.com

*U.S. dollar amounts are translated from yen at the rate of ¥150=U.S.$1, the approximate rate on the Tokyo Foreign Exchange Market on March 31, 2025.

About Institute of Science Tokyo

Institute of Science Tokyo (Science Tokyo) was established on October 1, 2024, following the merger between Tokyo Medical and Dental University (TMDU) and Tokyo Institute of Technology (Tokyo Tech), with the mission of "Advancing science and human wellbeing to create value for and with society."

About University of Tsukuba

University of Tsukuba was established in October 1973, due to the relocation of its antecedent, the Tokyo University of Education, to the Tsukuba area. As the new concept comprehensive university in Japan to be established under a country-wide university reform plan, the University has featured "Openness" with "New Systems for Education and Research" under a "New University Administration." The university reform plays a major role in our continuing effort for improvement. We are striving to create a unique, active, and internationally competitive university with superlative education and research facilities.

About Quemix Corporation

Quemix Inc., a consolidated subsidiary of TerraSky Co., Ltd. (Headquarters: Chuo-ku, Tokyo; CEO: Hideya Sato), conducts R&D in quantum computers, quantum sensors, and materials computation. Guided by its vision, "Realizing the Future Envisioned through Quantum Technology," Quemix's mission is to enable breakthrough innovations for companies leading the quantum era.

Since its establishment in 2019, Quemix has specialized in developing algorithms for Fault-Tolerant Quantum Computers (FTQC). The company developed and patented the Probabilistic Imaginary-Time Evolution (PITE®) algorithm, which has been mathematically proven to achieve quantum speedup in quantum chemistry calculations. As Japan's pioneer in FTQC algorithms, Quemix aims to bring practical quantum computing applications to materials computation and simulation by 2028.

Media Inquiries

Mitsubishi Electric Corporation

Public Relations Div.

E-mail：prd.gnews@nk.MitsubishiElectric.co.jp

Institute of Science Tokyo

Public Relations Division,

E-mail：media@adm.isct.ac.jp (Group)

University of Tsukuba

Bureau of Public Relations

E-mail：kohositu@un.tsukuba.ac.jp

Quemix Corporation
TerraSky Co., Ltd. – PR Contact
E-mail：pr@terrasky.co.jp

Customer Inquiries

Mitsubishi Electric Corporation Advanced Technology R&D Center
https://www.MitsubishiElectric.com/ssl/contact/company/rd/form.html
https://www.MitsubishiElectric.com/rd/