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Developing 3D Models of Atom-Like Defect Spin Memories in Crystals for Quantum Technology Research and Education

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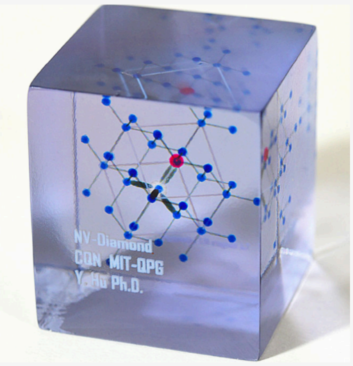
ABSTRACT: The development of quantum technologies, including quantum computers and networks, requires entanglement distribution across individually controllable qubits. Color centers in diamond and silicon are leading solid-state qubits, so-called "artificial atoms". Artificial atoms have been demonstrated for on-demand remote entanglement, coherent control of ancillary qubits with minute-long coherence times, and memory-enhanced quantum communication. There is an open need for clear and intuitive visualization of artificial atoms for research and education alike. Here we introduce a new visualization tool based on polyjet 3D printing technology to create detailed multimaterial multicolored 3D models of atomic defects, specifically focusing on color centers in diamond and silicon. These models accurately represent the defect structures in a hand-held form (less than 2 in.). We leverage the printer's capability to deliver realistic patient-specific models with multiple materials on the same production run. This approach enhances quantum technology education by offering interactive tools and early introduction of quantum concepts in K-12, fostering a quantum-literate future generation.



KEYWORDS: *Color Centers, Diamond, Silicon, Solid-State Qubits, 3D Printing, Quantum Technology*

■ INTRODUCTION

Quantum technology is crucial for advancing secure communication, powerful computation, and precision measurements.[1−4] Across various quantum technology platforms-including trapped ions, superconducting circuits, quantum dots, and color centers-understanding the underlying quantum phenomena is critical for the development of robust quantum systems. Among these platforms, color centers show significant promise due to their potential for stable and coherent quantum memories and repeaters, which are the foundation of emerging quantum networks.[2−4] Quantum Internet is needed over classical Internet for its unparalleled security through quantum key distribution, faster communication and data processing via quantum entanglement and superposition and enabling new applications like quantum computing and quantum sensing. Figure 1 shows a schematic of a future color center-based quantum network across the United States, highlighting long-distance quantum communication. In this quantum network,[2] qubits replace classical bits, allowing information to exist in multiple states and enabling entanglement for secure, efficient communication. The network connects three nodes (Alice, Bob, and Charlie) using fiber optics and qubit-based links, demonstrating robust quantum information transfer over large distances. Quantum memories, such as the one depicted at Bob's node, store quantum information temporarily, enabling complex operations like entanglement swapping and error correction. Quantum repeaters, positioned between nodes like Alice and Charlie, extend the communication range by maintaining entanglement and coherence over long distances, thus overcoming the limitations of direct transmission. Additionally, color centers play a crucial role in quantum sensing, providing high sensitivity and precision for measuring physical quantities, which is essential for various applications in quantum technology. Physical models for these atom-like defect spin memories in crystals, particularly in diamond and silicon,[5,6] are essential as they hold significant potential for propelling both research and educational endeavors in quantum technology. Traditional approaches to 3D modeling of atomic structures have primarily focused on molecules and bulk crystals.[7−10] However, modeling the atomic defects in crystals, especially the group IV-vacancy color centers crucial for quantum networks (Figure 1), demand a specialized approach. Current visualization techniques fall short in capturing the detail of these defects, creating a gap that hinders both academic understanding and practical advancements in quantum technology. Recognizing this, our study aims to bridge this gap by leveraging the capabilities of advanced 3D printing technology.[11]

Our project utilizes advanced 3D-printed models to illuminate the complex effects of orientation and symmetry variability on the magnetic and optical properties of color centers in quantum materials. By using the 3D models of

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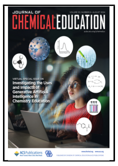

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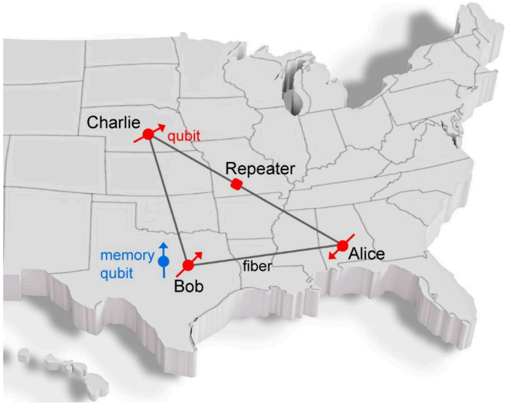
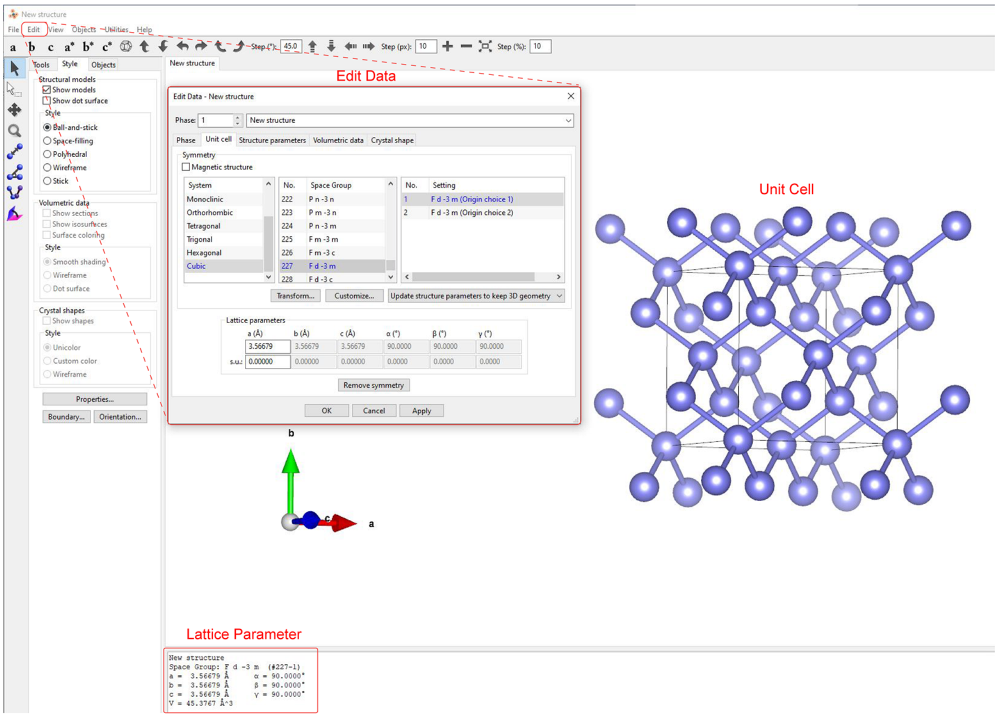


Figure 1. Schematic of a future quantum network across the United States. This diagram shows a plan for a future quantum network that connects different locations across the country. In this network, we have three people: Alice, Bob, and Charlie. They represent different locations that are part of the network: Alice, Bob, and Charlie are like different "computers" or "stations" that can communicate with each other using special "quantum bits" (qubits), which are used to send and process information. Bob has a special tool called a "memory qubit" that helps him keep information safe for a short time. This helps him manage the communication between Alice and Charlie by temporarily storing and sending information. A quantum repeater is a device that helps extend the distance between Alice and Charlie, so they can stay connected even over long distances. Optical fibers (gray lines) are like invisible "highways" that carry information between Alice, Bob, and Charlie using light. The network uses special color centers in diamonds and silicon, which are known for their ability to store and transmit information very effectively. This setup shows how these key components-qubits, memory qubits, repeaters, and optical fibers-work together to make advanced quantum communication possible.

nitrogen-vacancy (NV) and Group IV color centers, students will benefit from enhanced visual and tactile learning to better understand the properties of these color centers. These 3D models allow students to physically manipulate and observe different orientations and symmetry of color centers such as NV and Group IV centers. By engaging with these models, students will gain an understanding of why these color centers have the properties they do, such as sharp zero-phonon lines, spin states, and hybridization of lattice atoms. They will learn about another application of the hybrid orbital picture of bonding, which is used to describe the bonding in these color centers. Students can see how nearby color centers in a crystal can interact with one another. They will use the 3D models to learn the interactions of nearby color centers, estimation of electric field magnitudes, and their implications for spin coherence. This active exploration bridges the gap between theoretical quantum mechanics and practical technological applications, fostering deeper comprehension and innovative problem-solving skills. The ability to visualize and manipulate these orientations directly helps demystify the underlying quantum mechanics involved, making this complex subject more accessible and engaging, thus preparing students for advanced studies and careers in the burgeoning field of quantum technologies.

We present a new method that merges modern 3D printing precision with the science of quantum mechanics. Our approach has enabled us to create detailed, multimaterial, and multicolored 3D models of atomic defects, specifically focusing on color centers in diamond and silicon. These models serve as educational tools that provide vivid and accurate representations of defect structures in a compact, hand-held size. Their small size not only saves costs and space but also makes learning more interactive and accessible, allowing for hands-on exploration and a deeper understanding of complex concepts. We offer a new platform for researchers, educators, and students to visualize and interact with the quantum world.

We developed a method for creating visualization models using VESTA and Blender, two open-source software tools.[12,13]



Step (°): 45.0 Step (px): 10 Step (%): 10

Edit Data - New structure

Phase: 1 New structure

Phase | Unit cell | Structure parameters | Volumetric data | Crystal shape

Symmetry

☐ Magnetic structure

System
Monoclinic
Orthorhombic
Tetragonal
Trigonal
Hexagonal
Cubic

No.	Space Group
222	P n -3 n
223	P m -3 n
224	P n -3 m
225	F m -3 m
226	F m -3 c
227	F d -3 m
228	F d -3 c

No.	Setting
1	F d -3 m (Origin choice 1)
2	F d -3 m (Origin choice 2)

Update structure parameters to keep 3D geometry

Lattice parameters

	a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)
	3.56679	3.56679	3.56679	90.0000	90.0000	90.0000
s.u.:	0.00000	0.00000	0.00000	0.0000	0.0000	0.0000

```
New structure
Space Group: F d -3 m  (#227-1)
a =  3.56679 Å       α = 90.0000°
b =  3.56679 Å       β = 90.0000°
c =  3.56679 Å       γ = 90.0000°
V = 45.3767 Å^3
```

Figure 2. Design unit cell 3D model with Vesta.

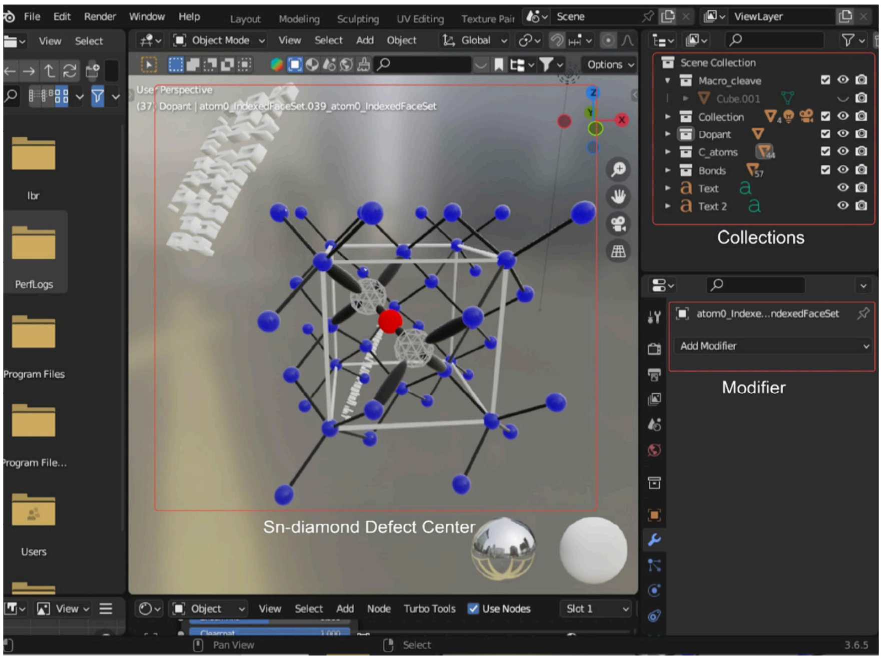


Figure 3. Creation of a 3D model for a defect center using Blender, with the Sn-diamond defect center displayed as a representative example.

We guide users through the process of crafting 3D models, from designing the unit cell in VESTA to finalizing in Blender. This democratizes the process of creating educational models and enhances the accessibility of quantum education. We improved model clarity by embedding the color center model inside a clear cube support. We resolved issues of nontransparency through an iterative process of sandpaper polishing and specialized coating. This ensures that each model serves as a clear window into the quantum world.

The impact of this endeavor is multifold. By enhancing the understanding and visualization of quantum defect centers, we not only pave the way for a broader appreciation of the complexities and possibilities inherent in quantum technologies but also ensure that these educational models are understandable, easily accessible and cost-effective. This approach allows students and researchers, even before reaching college, to engage with and contribute to the field of quantum technology in a more tangible and affordable manner. As a result, this work represents a significant step toward a future where quantum technologies are more widely appreciated and utilized, ushering in a new era of scientific education and technological advancement.

■ PROCEDURE

Design Unit Cell 3D Model

To create a 3D model for a color center, we use VESTA to construct the unit cell (Figure 2). We chose the diamond color center as our primary model for discussion and representation because its crystal structure is similar to silicon, except for the lattice constants and types of atoms.[14] To generate a new structure, input the crystallographic details in the 'Edit Data' section. Use lattice parameters a, b, c at 3.56679 Å and angles α, β, γ at 90.0000°, along with the space group $Fd\bar{3}m$ (#227).[15] We also adjust the model's bond thickness and atomic dimensions. This establishes a solid foundation for the next stage, where we transfer the structure to Blender to add complexities of the defect center. The crystal structure data is exported as a VRML (.wrl) file after the model is created.

Creation of 3D Models for Defect Centers

Importing the.wrl file into Blender preserves each atomic element, bond, and the unit cell frame as distinct subobjects, enabling precise and detailed modifications.[16] As shown in Figure 3, Blender's subobjects can be easily navigated to modify the diamond structure, tailoring them to represent specific atomic configurations of various color. Blender's modifier is used for accurately depicting the unique crystal structure of color centers. Additionally, desired text could also be added to the label or provide further details on the model. To ensure the stability of the printed defect model, we also incorporate a clear cubic structure to serve as a support and protective framework.

Figure 4 presents a visual representation of different color centers designed in Blender, each illustrating a distinct type of atomic defect within crystal structures. The NV-diamond model is displayed in Figure 4a, showcasing a single unit cell with NV centers.[17,18] These centers form when a nitrogen atom replaces a carbon atom adjacent to a vacancy in the diamond lattice. The defect structure of NV centers creates a localized electronic state, making them highly sensitive to magnetic fields and ideal for high-precision sensing and quantum computing at room temperature. In Figure 4b, a Sn-diamond model is shown,[19,20] where tin atoms replace two carbon atoms in the lattice, forming "SnV" centers. The substitutional Sn atoms adjacent to two vacancies create a defect with unique electronic and optical properties that are different from the NV color centers. The narrowband photon emission properties and high quantum efficiency in these SnV are crucial for creating indistinguishable photon sources in quantum networks. The Si-diamond structure in Figure 4c, with a 1 × 2 unit cell structure, contains two adjacent unit cells, each with a silicon vacancy center (SiV).[21] The SiV center is formed by replacing two neighboring carbon atoms in the diamond matrix with a silicon atom. SiV centers are highly desirable for scalable quantum photonics due to their symmetrical electronic properties and stable, bright optical

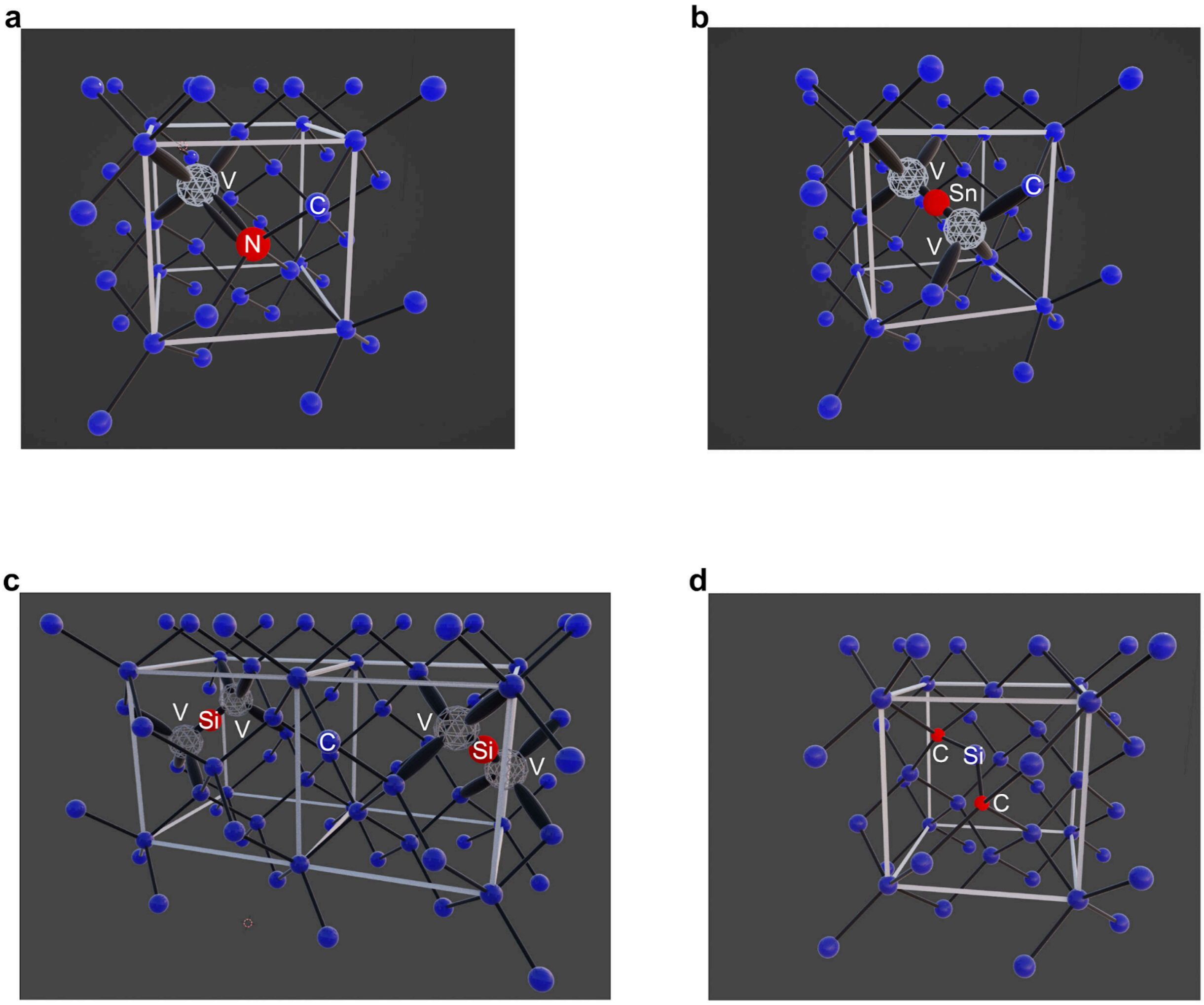


Figure 4. 3D representations of the designed defect center models. (a) NV color center in diamond (1 × 1 unit cell); (b) SnV color center in diamond (1 × 1 unit cell); (c) SiV color center in diamond (1 × 2 unit cell); (d) G center in silicon (1 × 1 unit cell). The text and support cubic structures are hidden for clear visualization. V represents vacancy.

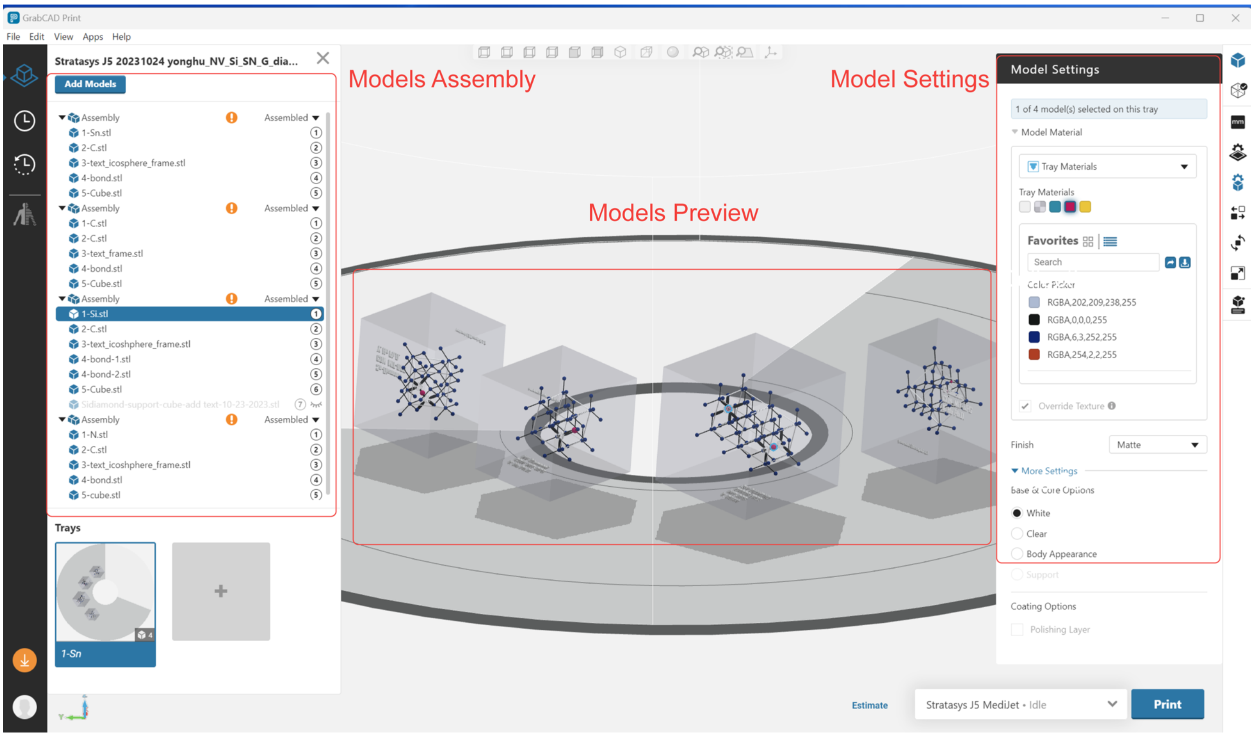
emissions. The G center in silicon, which is a defect consisting of a pair of substitutional carbon atoms bonded to a silicon self-interstitial within the silicon crystal lattice, is shown in Figure 4d. G centers are particularly noted for their sharp zero-phonon lines and are considered promising candidates for solid-state quantum emitters due to their long coherence times and compatibility with existing semiconductor technologies. Each of these color centers' unique formation mechanisms endow them with distinct electronic and photonic properties, making them invaluable for various quantum information processes, such as qubit operation, quantum communication, and sensing. These 3D models provide an invaluable educational resource, offering a clear and tangible way to visualize and understand the complex atomic structures and the formation processes of these color centers, thereby enhancing the comprehension of their properties and applications in the field of quantum information science.

3D Printing Color Center Models

To prepare models for 3D printing, export each element group - atoms, defect structures, bonds, clear support cubes, and text labels - into individual STL files. After preparing all separate STL files, in GrabCAD Print click File and choose "Add as assembly" to import all STLs with the same origin (Figure 5). The assembly process is repeated for each color center models' group of STL files. Adjust the percentages equally to maintain 3D proportions until you obtain desired dimensions.

After assembly, the model settings are fine-tuned. To ensure a clear and distinctive representation of each segment, specific colors are assigned to each component, including atoms, defect structures, bonds, support cubes, and text labels. This work used various Vero materials, and for optimal post-processing appearance, adjust the Finish setting to Matte and set "Base & Core Options" to white for all components except the clear support cube, which should be transparent and have the highest priority in the model components list. Use GrabCAD's "Arrange this tray" option and orient each model by 45 deg around the X and Y axes to minimize layering impact and enhance internal visibility. These preparations ensure a 3D model accurately illustrating the atomic structures of color centers in diamond, with an estimated printing time of approximately 10 h.

Figure 6 displays 3D previews of the completed defect center models. Each model is embedded within a clear cube along with detailed text annotations to describe the model. This figure shows the final result of our 3D printing process. It demonstrates the accuracy and clarity with which we can produce complex color centers. This provides a useful tool for enhancing the comprehension of quantum structures in research and education.



Stratasys J5 20231024 yonghu_NV_Si_SN_G_dia...

- Assembly — Assembled
  - 1-Sn.stl ①
  - 2-C.stl ②
  - 3-text_icosphere_frame.stl ③
  - 4-bond.stl ④
  - 5-Cube.stl ⑤
- Assembly — Assembled
  - 1-C.stl ①
  - 2-C.stl ②
  - 3-text_frame.stl ③
  - 4-bond.stl ④
  - 5-Cube.stl ⑤
- Assembly — Assembled
  - 1-Si.stl ①
  - 2-C.stl ②
  - 3-text_icoshphere_frame.stl ③
  - 4-bond-1.stl ④
  - 4-bond-2.stl ⑤
  - 5-Cube.stl ⑥
  - Sidiamond-support-cube-add text-10-23-2023.stl ⑦
- Assembly — Assembled
  - 1-N.stl ①
  - 2-C.stl ②
  - 3-text_icoshphere_frame.stl ③
  - 4-bond.stl ④
  - 5-cube.stl ⑤

Model Settings

1 of 4 model(s) selected on this tray

Model Material: Tray Materials

Favorites

Search

Color Picker
- RGBA,202,209,238,255
- RGBA,0,0,0,255
- RGBA,6,3,252,255
- RGBA,254,2,2,255

☑ Override Texture

Finish: Matte

More Settings

Base & Core Options
- ● White
- ○ Clear
- ○ Body Appearance
- ○ Support

Coating Options
- ☐ Polishing Layer

Stratasys J5 MediJet • Idle

Figure 5. Screenshot of GrabCAD Print software settings. Each color center is imported as a separate assembly, with materials and color settings individually applied to each part in the Model Settings. The preview shows the model post-application of these settings. The cubes printed for this demo were approximately 2 in. in X, Y, and Z.

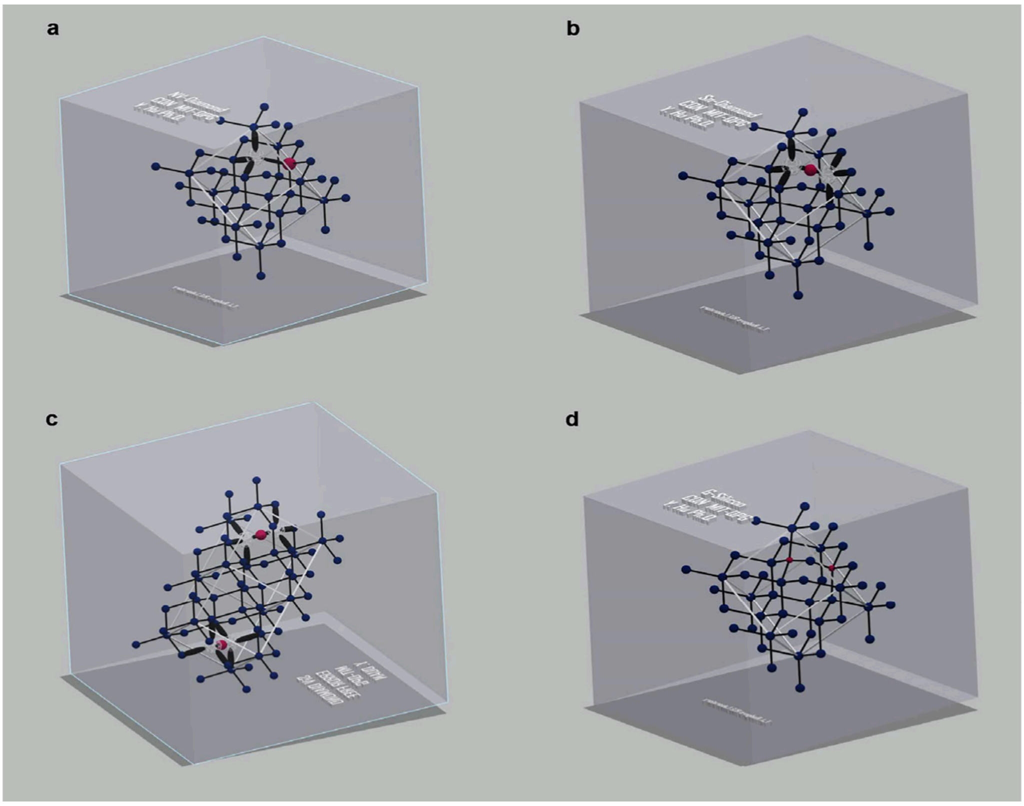


Figure 6. 3D previews of printed color center models with clear supports and labels. (a) NV color center in diamond; (b) SnV color center in diamond; (c) SiV color center in diamond; (d) G center in silicon. Each model includes clear cubic supports and text annotations, showing the final print configuration.

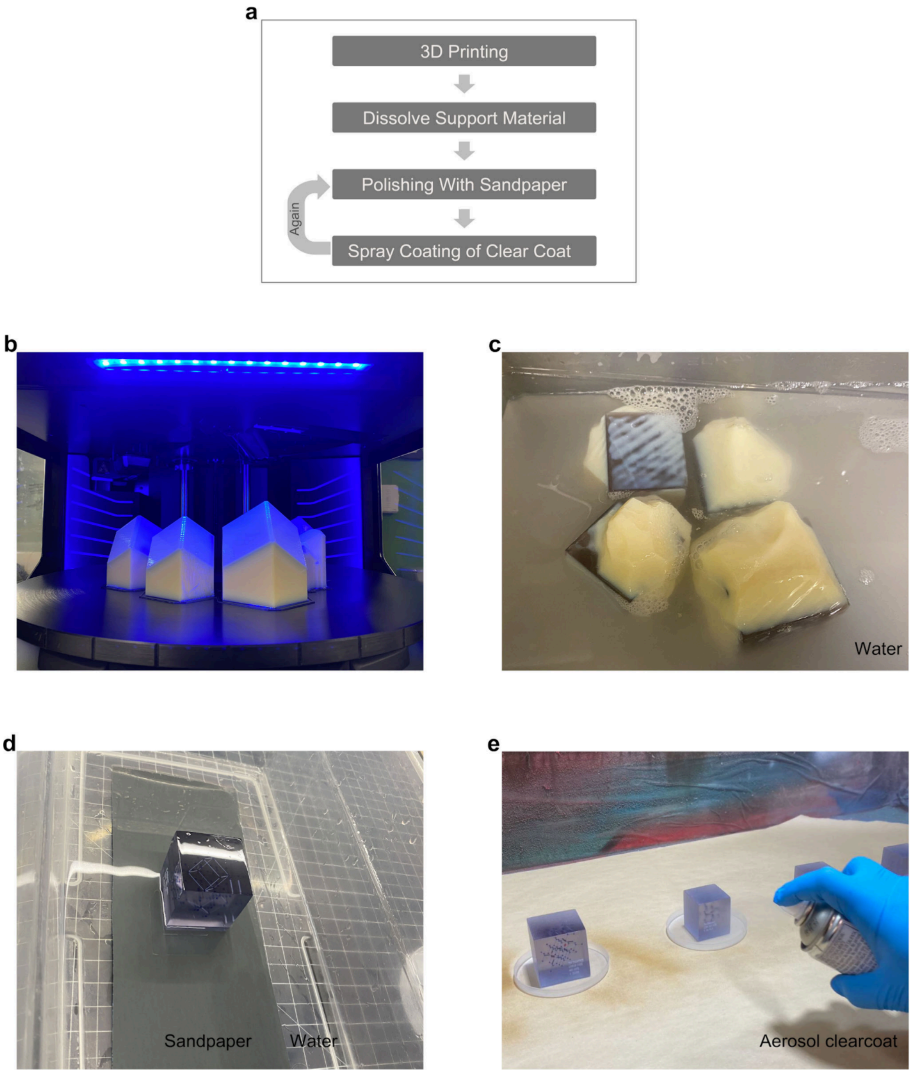


Figure 7. Post-processing for 3D-printed color center models. (a) Post-processing flowchart. (b) Printed color center mode inside the support materials with a Stratasys J5 printer. (c) Dissolving the printed model in water. (d) Polishing the printed model with sandpaper of 1200, 2000, and 300 grit. (e) Spray coating of printed mode (after sanding) with Spray Max 2K glamour high gloss aerosol clear (368 0061).

Post-Processing for 3D-Printed Color Center Models

Figure 7a shows the 3D printing process as well as post-processing steps. Figure 7b displays the model emerging from the printer, encased in water-soluble WSS150 support material. Although structurally sound, this initial form requires meticulous post-processing to reveal the intricate color center structures it encapsulates. After printing, the model is detached from the build tray carefully using a scraper or spatula. Immerse the model in water for 2 days, stirring and replacing the water occasionally (Figure 7c). To ensure complete removal of the supports, replace the water five times. The initial surface is rough, which initially obscures the internal detail. The roughness of the surface is intentional to enable a consistent finish on all faces and is generated by microscopic intrusion of the support material into the clear material. By starting with the same surface finish on all sides, we ensure that the same polishing process on all sides will result in the most consistent polish on all sides. To obtain glass-like clarity, we employ wet polishing and finish with a durable two-part polyurethane coating as shown in Figure 7d. After sanding, apply a spray coat (Figure 7e) to protect the model from environmental factors and enhance its transparency.

Figure 8 shows the clear 3D printed model resulting from this process. The crystal structure is now vivid, with each atomic and defect structure sharply defined. It serves as a tangible and visually striking educational tool. Its clarity and precision make it an ideal resource for those who want to understand quantum structures better. It provides a real-world representation of concepts that are often difficult to visualize.

Enhancing Quantum Engineering Education with 3D-Printed Models: Insights from MIT's Laboratory Course

In the Spring of 2024, our exploratory study conducted within the "6.2410 − Laboratory in Quantum Systems Engineering: Quantum Engineering Platforms" course at MIT, using the 3D-printed models to enhance the explanation of the properties of color centers through tactile and visual learning. The course included a detailed module focused on the orientation-dependent magnetic field sensing capabilities of NV centers in diamonds. Through hands-on experiments, students examined how the orientation of these NV centers affected their quantum properties. The setup included diamonds embedded with NV centers, magnets for generating variable magnetic fields, and a photodetector to capture changes in fluorescence emission. This

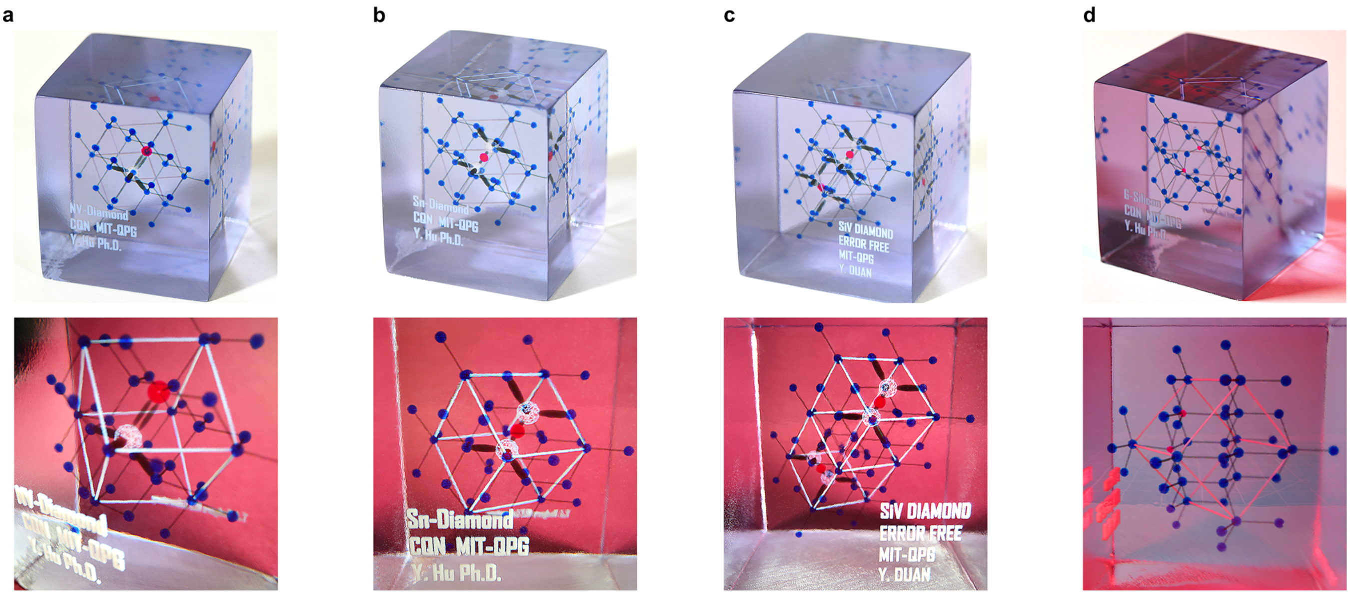


Figure 8. Optical images for 3D printed color centers after post-processing. (a) NV color center in diamond (size: 1.72 × 1.72 × 1.84 (H) inch); (b) SnV color center in diamond (size: 1.72 × 1.72 × 1.84 (H) inch); (c) SiV color center in diamond (size: 1.72 × 1.72 × 1.84 (H) inch); (d) G center in silicon (size: 1.88 × 1.88 × 2.06 (H) inch).

experimental setup allowed students to analyze the impact of magnetic field orientation on NV center fluorescence both visually and quantitatively, linking theoretical quantum mechanics concepts to real-world applications in quantum sensing. Additionally, the course facilitated in-depth discussions on the structural and environmental sensitivity differences between NV centers and Group IV color centers, such as SiV and SnV centers in diamond, and G centers in silicon. These discussions explored the minimal environmental sensitivity of centers like SiV and SnV, making them suitable for applications requiring long coherence times and sharp emission lines.

Our 3D models provided students with a comprehensive understanding of various quantum concepts, including:

- The relevance of sharp zero-phonon lines through the Debye–Waller factor, illustrating the static lattice of NV defects and the resulting sharp emission lines suitable for quantum technologies.
- How color center fluctuations correlate with emission line broadening and spin coherence times.
- Spin states, hybridization of lattice atoms, nitrogen defect atoms, and vacancies, providing detailed discussions on hybridization states, valence electron distribution, and their impact on spin coherence and quantum technology suitability.
- Main decoherence sources in NV systems. The models provide a visual and tactile means to examine the main sources of decoherence in NV systems, such as Carbon-13 nuclear spin hyperfine interaction and paramagnetic spin defects like nitrogen-14. By demonstrating the effects of Carbon-13 purification and the role of paramagnetic defects, students gain a deeper understanding of how these factors influence decoherence channels.
- Visualizations of distances between NV vacancies and estimation of electric field magnitudes, highlighting the impact of fluctuating electric fields caused by phonon interactions on spin coherence, enabling students to grasp the distances and electric fields between color centers and their implications for quantum coherence.

Feedback from the students was overwhelmingly positive, with many noting that the 3D models enhanced their understanding of material properties and quantum technologies (ed4c00343_si_002.pdf). They particularly appreciated the interactive nature of the experiments and the clear, tangible connection between the models and complex quantum concepts. Suggestions for future courses included the addition of more diverse quantum materials and detailed annotations to the models to further aid in the comprehension of the intricate details of quantum material behavior. This innovative educational approach not only deepened students' understanding of advanced quantum phenomena but also stimulated a heightened interest in further quantum technology research and applications. The success of this module underscores the potential of integrating practical, tactile learning tools into the study of sophisticated scientific topics, making them more accessible and engaging for the next generation of scientists and engineers.

■ DISCUSSION

Going forward, we can create educational materials around these 3D models, including simulations of spin entanglement using internal mechanisms connected by Bluetooth, museum exhibits, and larger crystal representations. Developing educational resources based on these models will significantly contribute to the understanding and advancement of quantum networks.

Proposal for future work:

- Develop more advanced 3D models to represent a wider range of atomic defects, expanding the scope of quantum network research.
- Integrate interactive components, such as LEDs for visualizing emissions, magnetic needles, or gyroscopic tops for spin states, and painted electronic orbitals to enhance the educational value of the models.
- Create a comprehensive quantum network curriculum that incorporates 3D models, simulations, and hands-on activities to train the next generation of quantum researchers and engineers.

- Investigate the potential for augmented reality (AR) or virtual reality (VR) applications in conjunction with the 3D models to provide immersive learning experiences.
- Collaborate with museums, science centers, and educational institutions to develop exhibits and demonstrations that showcase the 3D models and their relevance to quantum networks.
- Show emitters embedded within cavity interfaces, such as 1D photonic crystal cavities in diamond.
- Explore the use of machine learning and artificial intelligence algorithms to automatically generate 3D models of atomic defects based on experimental data, accelerating the research-to-modeling pipeline.
- Evaluate the impact of the 3D models and associated materials on student learning, research progress, and public understanding of quantum networks, using this information to guide future initiatives.

CONCLUSIONS

We have successfully demonstrated the potential of 3D-printed models to visualize and understand atomic defects in quantum networks, specifically focusing on color centers in diamond and silicon. Employing advanced 3D printing alongside open-source software, we've created detailed, multimaterial, and multicolored models that serve as educational tools. This innovative approach has significantly enhanced comprehension of complex atomic structures, bridging the gap between abstract quantum phenomena and tangible understanding. The implications of this work extend beyond academic research to educational realms, providing a novel platform for inspiring and educating future generations in quantum technology. This endeavor not only advances the field of quantum system modeling but also sets a precedent for future developments in making quantum mechanics more accessible and comprehensible.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available at https://pubs.acs.org/doi/10.1021/acs.jchemed.4c00343.

3D files and project for replication, including the .wrl file from VESTA, the blender file for all color centers, and separate .stl files for each component, along with the 3D-printed project file in the printer (ZIP)

Survey of student perceptions of 3D-printed models in quantum technology education (PDF)

Step-by-step creation guide for creating the 3D models of color centers (PDF)

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Notes

The authors declare no competing financial interest.

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