

Introduction: Quantum Computing

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Quantum computing has entered a new era—an era where quantum coherence is no longer an elusive phenomenon observed only in specialized laboratories, but a working principle guiding the design of real devices, algorithms, and applications. The 2025 Nobel Prize in Physics, awarded to John Clarke, Michel Devoret, and John Martinis "for the discovery of macroscopic quantum mechanical tunneling and energy quantization in an electric circuit," captures this transition in a single, elegant stroke.^{1–3} The prize recognizes not just an experiment, but a shift in scientific imagination: the moment when quantum behavior, once confined to the microscopic scale, was coaxed into the macroscopic realm of circuits and devices.^{4,5} That discovery laid the foundation for superconducting qubits and, with them, the modern quantum computer.^{6–14}

It is remarkable to consider how swiftly this field has evolved.¹⁵ In less than a decade, what began as fragile, few-qubit prototypes has matured into multiqubit processors that can execute thousands of entangling operations with measurable fidelity. Alongside these hardware advances, the algorithmic, chemical, and physical sciences have converged in ways that few could have predicted.^{16,17} The language of "gates" and "circuits" now mingles effortlessly with that of "wavefunctions" and "correlation." The experimentalist's qubit calibration routine has become as vital to progress as the theorist's Hamiltonian decomposition. Quantum computing, once a thought experiment, has become a shared experiment—one conducted by physicists, chemists, engineers, and computer scientists alike.

This collection on Quantum Computing reflects that integration. The six reviews gathered here are not isolated commentaries but interconnected chapters of a single narrative: the transformation of quantum mechanics from fundamental science to functional technology. Each article illuminates a layer of the "quantum stack"—from the physics of open quantum systems and gate fidelity to the architectures, algorithms, and applications that together define the road to scalable quantum advantage.

THE QUANTUM FRONTIER: FROM OPEN SYSTEMS TO REAL DEVICES

Every qubit is a conversation with its environment, and understanding that dialogue is central to progress. In *Quantum Algorithms and Applications for Open Quantum Systems*, Kowalewski and co-workers address the challenge head-on: how to design quantum algorithms that thrive, not collapse, in the presence of dissipation and decoherence. By uniting

theoretical constructs such as Lindblad equations and non-Markovian baths with algorithmic tools like quantum jump trajectories and variational solvers, they outline strategies that make noise not just tolerable, but instructive. Their work reminds us that every realistic quantum device is an open system and that embracing rather than ignoring this fact may lead to more robust algorithms and more predictive models for chemistry, biology, and materials.

MEASURING, DIAGNOSING, AND MASTERING ERROR

Progress in quantum computing is inseparable from progress in measurement. In *Benchmarking Quantum Gates and Circuits*, Emerson and colleagues take readers on a tour through the intricate landscape of quantum error characterization. Randomized benchmarking, process tomography, cross-entropy tests, and emerging deterministic methods each serve as diagnostic instruments in the experimentalist's toolkit. But benchmarking is more than a calibration protocol—it is a language of accountability, a way to translate the imperfections of physical qubits into actionable metrics. Their review illustrates how carefully designed benchmarking experiments can reveal the hidden anatomy of noise, guiding the design of both hardware and error correction strategies. As the field advances, the authors argue, benchmarking will become not merely a report card, but a feedback loop—where measuring, modeling, and mitigating errors form a continuous cycle of improvement.

TOWARD FAULT-TOLERANT QUANTUM COMPUTATION

If benchmarking is the microscope of quantum computing, then error correction is its immune system. In *Quantum Error Correction and Mitigation: Pathways Toward Fault-Tolerant Computation*, Terhal, Preskill, and coauthors explore the architecture of that system in exquisite detail. They map the terrain of quantum codes—from the planar geometry of surface codes to the infinite-dimensional landscapes of bosonic and cat codes—and analyze how these mathematical constructs can be made physically real. Their review does

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not stop at the asymptotic limit of fault tolerance; it also surveys pragmatic strategies for the noisy present, such as zero-noise extrapolation and probabilistic error cancellation. The story they tell is one of balance: between overhead and resilience, between theory and implementation, between the ideal of logical qubits and the reality of their imperfect ancestors.

QUANTUM CHEMISTRY AND MATERIALS AT THE EDGE OF FEASIBILITY

Among the most compelling motivations for quantum computing is its promise to revolutionize how we understand and predict molecular behavior. In *Quantum Simulation for Chemistry and Materials Science*, Reiher and co-workers bring this promise into focus. They examine how molecular Hamiltonians and spin models can be translated into quantum circuits and how hybrid workflows—combining density functional theory, coupled cluster theory, and quantum routines—can reach chemical accuracy for systems beyond the reach of classical methods. Through examples ranging from small molecules to periodic solids, the authors delineate the metrics that matter most: qubit count, circuit depth, and the trade-offs between accuracy and feasibility. Their perspective situates chemistry not as a distant application but as a guiding compass for algorithmic and hardware design.

EMBEDDING, FRAGMENTATION, AND THE QUANTUM CHEMISTRY OF REALITY

Chemical systems are often too large and too complex for brute-force quantum simulation. *Multireference Embedding and Fragmentation Methods for Classical and Quantum Computers*, by Verma, Mitra, Wang, and Gagliardi, offers a conceptual bridge between the worlds of chemistry and computation. The authors trace the development of density matrix embedding theory (DMET) and localized active space (LAS) frameworks that partition complex systems into manageable fragments while preserving quantum entanglement across their boundaries. By extending these approaches to quantum computers—integrating DMET with variational quantum eigensolvers (VQE) and related hybrid algorithms—they show how the computational burden of multireference methods can be distributed across classical and quantum resources. Applications range from the dissociation of molecular bonds to the study of transition-metal centers and color centers in diamond. The review is both technical and visionary: it redefines how quantum advantage might first appear—not as a sudden leap in speed, but as a gradual broadening of the class of problems that can be solved with realistic precision.

BEYOND THE STANDARD MODEL OF QUANTUM COMPUTATION

The quantum landscape extends beyond qubits on chips. In *Emerging Paradigms for Quantum Computing: Architectures, Algorithms, and Applications*, Kim and collaborators explore frontiers that challenge the conventional gate-based model. Continuous-variable systems, photonic networks, analog simulators, and hybrid architectures are not mere detours—they are parallel evolutions, each probing a different balance of controllability, scalability, and physical intuition. Their review situates these platforms within a broader vision of modular, interconnected quantum systems capable of specialized computation and simulation. As the authors suggest, diversity

in architecture is not a weakness but a strength: the path to a quantum future may well be plural, with multiple technologies coexisting and complementing one another.

INTEGRATION, CODESIGN, AND THE ROAD AHEAD

What emerges from these six reviews is not a snapshot but a living landscape. Quantum computing today is defined by interplay—between physics and chemistry, hardware and theory, error and correction, imagination and implementation. It is a field in which progress depends not on isolated breakthroughs but on codesign: algorithms that respect hardware constraints, hardware that anticipates algorithmic needs, and applications that inform both.

From a policy and programmatic perspective, this collection underscores the need for integrative milestones. Benchmarks of chemical accuracy, robust open-system simulations, experimentally grounded error models, and hybrid workflows that bridge classical and quantum resources all represent meaningful steps toward practical quantum advantage. Just as the transistor revolution required a synthesis of materials science, electrical engineering, and computer architecture, the quantum revolution will demand collaboration across every layer of science and technology.

In celebrating this moment—when the physics of quantum tunneling has blossomed into the technology of quantum information—we are reminded that the story of quantum computing is, at its core, the story of coherence harnessed by creativity. The reviews in this collection invite the reader to engage not only with equations and circuits but also with the larger vision of what a quantum machine can mean: a new scientific instrument, a new form of computation, and a new way of understanding the physical world.

We hope this collection inspires curiosity and cross-pollination across disciplines. The quantum future will not arrive all at once; it requires vision and support, and it will be built piece by piece, qubit by qubit, experiment by experiment. And as these reviews show, that construction is already well underway.

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Notes

Views expressed in this editorial are those of the authors and not necessarily the views of the ACS.

Biographies

Prineha Narang is Professor of Physical Sciences and Electrical and Computer Engineering at the University of California, Los Angeles, where she holds the Howard Reiss Chair. She earned her B.S. in Materials Science from Drexel University and her Ph.D. in Applied Physics from Caltech, focusing on light–matter interactions and quantum plasmonics. After postdoctoral research at MIT, she joined Harvard University as Assistant Professor of Computational Materials Science before moving to UCLA in 2022. Narang’s research explores quantum materials, nonequilibrium dynamics, and quantum photonics, combining theory and computation to predict and control

light–matter interactions at the quantum level. Her group develops first-principles approaches to design materials for next-generation quantum and photonic technologies. Her honors include the Maria Goeppert Mayer Award from the APS, the Mildred Dresselhaus Prize, a Guggenheim Fellowship, and an NSF CAREER Award. A recognized leader in quantum science, Narang also serves on national advisory panels shaping U.S. research priorities in quantum materials and information technology.

Sabre Kais holds the Goodnight Distinguished Chair in Quantum Computing in the Department of Electrical and Computer Engineering at North Carolina State University (from 2024) and is also Professor (and Associate Faculty) in Chemistry and Adjunct Professor of Physics there. He earned his B.Sc. in Chemistry (1979–83) and M.Sc. (1983–84) from the Hebrew University of Jerusalem and his Ph.D. in Theoretical Chemistry from the same institution in 1989 under Prof. R. D. Levine and M. Cohen. After postdoctoral studies at Harvard University (with Dudley Herschbach) and elsewhere, he joined Purdue University in 1994 and held full professorship roles in Chemistry, Physics, Computer Science and Engineering until his move to N.C. State. His research spans quantum algorithms for chemistry, quantum machine learning for molecules and materials, quantum coherence and transport, and finite- and large-dimension scaling methods for electronic structure and critical phenomena. He is a Fellow of the American Physical Society and the American Association for the Advancement of Science, and his honors include the 2019 Herbert Newby McCoy Award at Purdue and a 2005 Guggenheim Fellowship.

Alan Aspuru-Guzik is a Professor of Chemistry and Computer Science at the University of Toronto, where he leads the Matter Lab and directs the Vector Institute's program in materials discovery. He received his B.S. and Ph.D. in Chemistry from the University of California, Berkeley, and completed postdoctoral research at Harvard University, where he later joined the faculty and established one of the earliest research groups in quantum computing for chemistry. Aspuru-Guzik's work spans quantum computing, machine learning, and automated materials discovery. His group develops algorithms and self-driving laboratory systems that accelerate molecular and materials design through artificial intelligence and quantum simulation. He is a Fellow of the American Physical Society, the Royal Society of Canada, and the Canadian Institute for Advanced Research (CIFAR). His honors include the Google Focused Research Award, the Canada CIFAR AI Chair, and the Canada Research Chair in Theoretical and Quantum Chemistry. Aspuru-Guzik is internationally recognized for pioneering the use of quantum computers for chemical simulations and for leading efforts toward autonomous, data-driven materials science.

Victor S. Batista is the John Gamble Kirkwood Professor of Chemistry at Yale University, where he has been a faculty member since 2001. He earned his B.Sc. in Chemistry from the University of Buenos Aires in 1989 and his Ph.D. in Theoretical Chemistry from Boston University in 1996. After postdoctoral research at the University of California, Berkeley, and the University of Toronto, he joined Yale's Department of Chemistry. Professor Batista's research focuses on theoretical and computational chemistry, with an emphasis on developing semiclassical and quantum dynamics methods to investigate photoinduced reactions, energy conversion, and catalytic processes. His group has published contributions to advancing the understanding of photosynthetic systems and the quantum control of chemical dynamics. As Director of the NSF Center for Quantum Dynamics on Modular Quantum Devices, Batista led a national effort to design quantum simulations of complex molecular systems using programmable Kerr-cat platforms. His recent work includes quantum

machine learning for drug discovery and quantum algorithms for simulating non-Markovian chemical dynamics. He is a Fellow of the Royal Society of Chemistry and an elected member of the Connecticut Academy of Science and Engineering.

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REFERENCES

- (1) Metz, C. "Google's quantum computer makes a big technical leap" *New York Times* Oct. 22 (2025).
- (2) Dutta, R.; et al. Simulating chemistry on bosonic quantum devices. *J. Chem. Theory Comput.* 2024, 20, 6426–6441.
- (3) Narang, P.; Hersam, M. C. From Macroscopic Quantum Tunneling to Quantum Computing: The 2025 Nobel Prize in Physics. *ACS Nano* 2025, 19, 37463–37464.
- (4) Chavez, J. et al. in APS Division of Atomic, Molecular and Optical Physics Meeting Abstracts F01. 027 (2023).
- (5) Chávez-Carlos, J.; et al. Driving superconducting qubits into chaos. *Quantum Science and Technology* 2025, 10, 015039.
- (6) Cao, Y.; et al. Quantum chemistry in the age of quantum computing. *Chem. Rev.* 2019, 119, 10856–10915.
- (7) Lanyon, B. P.; et al. Towards quantum chemistry on a quantum computer. *Nature Chem.* 2010, 2, 106–111.
- (8) Kyaw, T. H.; et al. Boosting quantum amplitude exponentially in variational quantum algorithms. *Quantum Science and Technology* 2024, 9, 01LT01.
- (9) Vu, N. P.; et al. A Computational Framework for Simulations of Dissipative Nonadiabatic Dynamics on Hybrid Oscillator-Qubit Quantum Devices. *J. Chem. Theory Comput.* 2025, 21, 6258–6279.
- (10) Smaldone, A. M.; et al. A hybrid Transformer architecture with a quantized self-attention mechanism applied to molecular generation. *J. Chem. Theory Comput.* 2025, 21, 5143–5154.
- (11) Wang, C. S.; et al. Efficient multiphoton sampling of molecular vibronic spectra on a superconducting bosonic processor. *Physical Review X* 2020, 10, 021060.
- (12) Wang, Y.; et al. Characterizing conical intersections of nucleobases on quantum computers. *J. Chem. Theory Comput.* 2025, 21, 1213–1221.
- (13) Cabral, D. G. A.; et al. A Roadmap for Simulating Chemical Dynamics on a Parametrically Driven Bosonic Quantum Device. *J. Phys. Chem. Lett.* 2024, 15, 12042–12050.
- (14) Lyu, N.; Bergold, P.; Soley, M. B.; Wang, C.; Batista, V. S. Holographic Gaussian Boson Sampling with Matrix Product States on 3D cQED Processors. *J. Chem. Theory Comput.* 2024, 20, 6402–6413.
- (15) Schleich, P. et al. *Quantum Computing for Quantum Chemistry* (American Chemical Society, 2025).
- (16) Wang, Y.; et al. Simulating open quantum system dynamics on NISQ computers with generalized quantum master equations. *J. Chem. Theory Comput.* 2023, 19, 4851–4862.
- (17) Lyu, N.; et al. Mapping molecular hamiltonians into hamiltonians of modular cqed processors. *J. Chem. Theory Comput.* 2023, 19, 6564–6576.