Quantum Computing Advantage in Energy

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Introduction

The global energy system is undergoing rapid transformation driven, *inter alia*, by decarbonization efforts, the shift to electrification, renewable integration, and increasing demands for scale, efficiency, and reliability. Managing this transition requires solving a growing set of computationally intensive problems spanning both **power grid** and **chemicals** (e.g., for fuels development) [1][2][3]. As energy systems become more interconnected and data-rich, a widening gap has emerged between the complexity of these challenges and the practical limits of existing computational tools [2][3][4].

Quantum computing introduces a fundamentally different computational model that may offer advantages for selected classes of problems central to the energy sector. Rather than replacing classical high-performance computing (HPC), advanced optimization, or machine learning, quantum approaches are best viewed as complementary tools that could address specific bottlenecks where classical methods face unfavorable scaling or rely heavily on approximation. While large-scale advantage will depend on hardware maturity, quantum computing is plausibly aligned with several of the most computationally demanding challenges in modern energy systems, making early exploration strategically relevant.

Certain Problems in Energy Push the Limits of Classical Computing

Power grid systems involve scale, nonlinearity, uncertainty, and strong interdependence, creating computational demands that stretch classical approaches to their limits [2][3][5]. As system size and realism increase, classical tools increasingly depend on heuristics, relaxations, and decomposition techniques that trade accuracy, coverage, or robustness for tractability [2][3][4]. Several examples illustrate these limits:

- **Power system optimization,** including optimal power flow (OPF), unit commitment, and dispatch planning, involves non-convex, mixed-integer, and nonlinear constraints that scale rapidly with grid size, renewable penetration, and operational complexity [2][5][6][7].
- **Predictive maintenance** requires extracting subtle signals from massive, high-dimensional sensor datasets, often in regimes where failure events are rare but costly [8][9][10].
- **Grid-load and renewable-generation forecasting** demands accurate representation and sampling of complex probability distributions with long-range temporal dependencies under significant uncertainty [3][10].

Chemical processes for energy depend on accurately modeling quantum-mechanical reaction pathways and thermodynamics that govern fuels, catalysts, and other energy-relevant chemicals. As reaction complexity increases—particularly for strongly correlated systems or processes operating across broad temperature and pressure ranges—classical simulation tools increasingly rely on approximations that limit predictive accuracy and scalability [4][11]. A representative example highlights these challenges:

- **Industrial chemical processes** depend on quantum-mechanical reaction pathways and thermodynamics that classical simulation tools approximate only crudely for large or strongly correlated systems [4][11].

  Note: For more information on a related class of challenges and use cases, please refer to the accompanying Industry Brief on Quantum Computing Advantage in Materials Science.

These bottlenecks share a common root: current computational methods are forced to approximate inherently complex or quantum-mechanical systems, leaving potential accuracy, efficiency, and insight unrealized [2][3][4].

Quantum Advantage in Energy

Quantum computers operate according to physical principles that directly model certain forms of complexity relevant to energy systems, including quantum-mechanical interactions, high-dimensional probability distributions, and rugged optimization landscapes [2][3][4]. This alignment suggests potential advantages for carefully selected subproblems where classical scaling is particularly unfavorable or approximation-heavy [2][4].

While theoretical results indicate that certain quantum algorithms may scale more favorably than classical approaches for sampling, simulation, or related tasks, translating these results into practical workflows for the energy sector depends on hardware quality, error rates, and problem-specific structure. As a result, early progress is expected to come from hybrid quantum–classical workflows, in which quantum subroutines augment specific components of existing pipelines rather than replace them outright [1][2][4][6].

High-Impact Examples Where Advantage May Emerge

While broad claims of quantum speedup should be treated cautiously, several high-value areas in energy stand out as plausible candidates for quantum advantage in the realm of **power grid:**

- **Power system optimization (OPF, unit commitment, dispatch planning):** Quantum optimization methods may complement classical solvers for selected subproblems within power system optimization, such as feasibility detection under nonlinear constraints, scenario-based sampling, or decomposition-based planning tasks [2][6][7]. As grids become more renewables-driven and operationally constrained, even incremental improvements in these components could reduce reserve requirements, curtailment, and congestion costs [2][6][7].
- **Predictive maintenance and fault detection:** Quantum-enhanced machine learning approaches have been proposed as a way to represent complex feature spaces for anomaly detection in large-scale sensor networks [8][10]. Incremental improvements in early fault detection could yield meaningful operational savings and reduce the risk of rare but catastrophic failures across energy infrastructure [8][9][10].
- **Grid-load and renewables-output forecasting:** Quantum generative models may eventually support more compact representation and sampling of complex, multi-scale probability distributions relevant to load and generation forecasting [3][10]. Improved scenario generation could help operators better plan around uncertainty, integrate renewables more effectively, and reduce balancing costs [3][10].

Beyond power grid applications, quantum computing’s potential in energy also extends to **chemical processes,** where long-standing challenges in reaction modeling and thermodynamics remain difficult for classical simulation tools.

- **Industrial chemical reaction modeling (thermodynamics and mechanisms):** Quantum computing is particularly well suited to simulating strongly correlated electronic structures that challenge classical quantum chemistry methods [4][12][13]. While achieving full chemical accuracy at industrial scale will require fault-tolerant systems, early hybrid workflows applied to smaller reaction fragments may provide improved insight into catalysts, reaction pathways, and decarbonization-relevant processes [4][12][13].

  Note: For more information on a related class of problems and use cases, please refer to the accompanying Industry Brief on Quantum Computing Advantage in Materials Science.

Across these areas, any early advantages are most likely to emerge through hybrid quantum–classical workflows that enhance existing optimization, simulation, and analytics pipelines rather than replace them wholesale.

Grand Challenges for Quantum Computing in Energy

As part of this Industry Brief Series, we have identified Grand Challenges relevant for different industries. By articulating these challenges, we hope to set a long-term direction for exploring quantum approaches and a clearer understanding of where future breakthroughs would translate into meaningful impact for various industries.

Power Grid: Quantum-Enabled N−1 Secure Chance-Constrained AC Unit Commitment

Achieving scalable, N−1 secure, chance-constrained optimization of power grid operations under full alternating-current (AC) physics represents a unifying grand challenge at the heart of quantum computing’s potential in power systems. As electricity grids integrate higher shares of variable renewable generation, operators must solve increasingly complex unit commitment and dispatch problems that combine non-linear power-flow constraints, mixed-integer decisions, contingency security requirements, and correlated uncertainty—pushing classical optimization tools toward heavy approximation and decomposition. Progress on this challenge would enable more robust, probabilistic grid scheduling that better anticipates contingencies and uncertainty, improving reliability while reducing reserve margins, curtailment, and operational inefficiencies. Importantly, advances in this area could support more resilient and flexible power systems as renewable penetration grows, while maintaining stringent reliability standards.

Chemicals: Accurate Reaction Thermodynamics Prediction for Industrial Chemical Processes

Achieving accurate, first-principles prediction of reaction thermodynamics for industrial chemical processes represents a unifying grand challenge at the heart of quantum computing’s potential in the energy sector. Many critical decarbonization pathways—spanning fuels, chemicals, and materials—depend on reliably estimating Gibbs free energy differences across a wide range of temperatures and pressures, a task that classical simulation tools can only approximate at scale. Solving this challenge would enable more confident in silico optimization of industrial reactions, reducing reliance on costly trial-and-error experimentation while accelerating the discovery of improved catalysts and process conditions. Importantly, progress in this area would translate directly into faster development cycles, lower energy intensity, and more efficient deployment of low-carbon technologies.

Why Executives Should Act Now

Organizations that engage early with quantum computing will be better positioned to shape emerging ecosystems, standards, and partnerships—advantages that are difficult for fast followers to replicate [14][15]. Access to specialized talent, hardware platforms, and domain-specific expertise remains limited and is increasingly concentrated among early movers [14][15].

Across the energy sector, leading firms and research organizations are already piloting exploratory quantum collaborations, signaling a gradual but meaningful shift toward experimentation [14][15]. Executives who invest now in partnerships, internal capability, and focused exploration will be better prepared for the inflection point at which quantum advantage begins to materialize.

How Executives Can Get Started

- Identify modeling, optimization, or forecasting workflows constrained by current computational limits
- Form cross-functional teams spanning engineering, data science, and strategy to assess quantum-relevant pain points
- Leverage IQMP resources to connect with quantum hardware providers, software developers, and academic researchers
- Launch small, well-scoped proof-of-concept projects to build organizational familiarity and technical readiness
- Promote awareness across technical and strategic teams of how quantum workflows may integrate with existing HPC and AI systems

Sources

1. A. Abbas, et al., “Challenges and Opportunities in Quantum Optimization,” Nature Review Physics, arXiv:2312.02279.

2. Morstyn, T. & Wang, X., “Opportunities for quantum computing within net-zero power system optimization,” Joule, 2024.

3. South Carolina Quantum & qBraid, “Quantum Computing for Energy Grid Optimization – White Paper,” 2025.

4. Hariharan, S., Kinge, S., & Visscher, L., “Modeling Heterogeneous Catalysis Using Quantum Computers: An Academic Industry Perspective,” Journal of Chemical Information and Modeling, 2025.

5. NREL – Connor O’Neil, “Quantum Computers Can Now Interface With Power Grid Equipment,” NREL News Feature, July 17, 2023.

6. IonQ, “IonQ and Oak Ridge National Laboratory Demonstrate Quantum Power Grid Optimization,” Press Release, July 31, 2025.

7. D-Wave & TNO, “Electrical Grid Optimization via Quantum Annealing,” Project Report, 2023.

8. Ajagekar, A. & You, F., “Quantum computing assisted deep learning for fault detection and diagnosis in industrial process systems,” Applied Energy, 2021.

9. Wang, D. et al., “Quantum-Enhanced Predictive Degradation Pathway Optimization for PV Storage Systems,” Energies, 2025.

10. Strata, F. et al., “Quantum machine learning early opportunities for the energy industry: A scoping review,” Frontiers in Quantum Science and Technology, 2025.

11. Paudel et al., “Quantum Computing and Simulations for Energy Applications,” ACS Engineering (2022).

12. Grimsley et al., “An adaptive variational algorithm for exact molecular simulations on a quantum computer,” Nature Communications (2019).

13. Sarkar et al., “Quantum Simulations of Chemical Reactions: Achieving Accuracy with NISQ Devices,” arXiv:2503.12084.

14. Massera Winigah & K. Etcheverry, “Quantum Computing in the Energy Sector,” Hello Tomorrow, Nov. 13, 2025.

15. Higgins, H. & Florizoone, P., “Quantum is coming: 2025 Quantum Readiness Index,” IBM Institute for Business Value, 2025.