Press Release

A Quantum Leap into a New Era of Materials Research

Algorithmiq and Fraunhofer ISC to Collaborate in Quantum Computing for Materials Development

Affordable medicine, rising energy costs, and dependence on strategic raw-material sources make new materials central to many questions. Traditional materials development is time-consuming and often takes years. Fraunhofer ISC is therefore pursuing accelerated development approaches - "Materials Acceleration" - based on digital methods, machine learning, and artificial intelligence. Additional acceleration and a broader exploration of the materials space are expected from quantum computers. The Italian company Algorithmiq, with proven expertise in quantum computing, has signed a memorandum of understanding (MoU) with Fraunhofer ISC to deepen this collaboration.

Fraunhofer ISC brings extensive experience in the chemical synthesis of a wide range of materials. Yet classical lab syntheses are time-consuming: developing a new material approach requires numerous experiments before the desired properties are achieved. Digital methods offer a path to faster development. By simulating and calculating structure-property relationships, unsuitable candidates can be screened out early and promising material options identified more efficiently. The underlying processes are highly complex: fully describing the dynamics of quantum many-body systems often demands extremely long compute times, even on today's supercomputers. Quantum computing could, for example, substantially speed up the quest for resource-efficient high-performance magnetic materials ("rare-earth-lean magnets" or "gap magnets") and enable deeper exploration of the materials space than ever before.

Quantum computing - accelerating exploration of the materials space

Algorithmiq is a Milano-based quantum computing company that specializes in developing quantum-native algorithms for drug discovery and molecular simulation. Its core aim is to compute molecular properties and dynamics far more accurately and efficiently than possible with classical simulations (e.g., classical quantum chemistry or molecular dynamics simulations). To ensure that these quantum algorithms - tailored to chemical and life-science questions - work on today's imperfect quantum computers, the team employs hybrid approaches in which a classical computer and a quantum computer collaborate: the quantum processor handles difficult quantum effects in molecules, while the classical computer oversees

optimization and data analysis. The methods are designed to exploit typical patterns in chemistry to yield reliable insights despite hardware errors.

Algorithmiq's life-sciences–oriented quantum computing concept won a $2 million Wellcome Leap prize in April for "the first demonstration of a fully quantum-classical workflow to simulate complex therapies and thus open a credible path to near-term quantum advantage in the life-sciences field." The team now aims to apply this concept to chemical materials development. To this end, they have entered into a strategic partnership with Fraunhofer ISC, leveraging Fraunhofer ISC's expertise in chemical materials synthesis and digitalization.

Solving complex problems more efficiently

"First, simulations can help identify our 'white spots' in the materials space more easily -materials we may not have been explicitly looking for, but whose properties could be highly promising," explains Prof. Dr. Miriam Unterlass, director of Fraunhofer ISC, outlining the goals of the collaboration. Another objective is to better understand the materials space through simulations and to find new solutions more quickly. "In the future, too, we will need the creativity of researchers to drive societally relevant innovations. Yet the toolkit will become more digital, and alongside real-world synthesis, the digital twin will gain great significance, allowing predictions of materials synthesis, product properties, and recycling outcomes across the entire product life cycle without having to trace every laboratory step." The integration of quantum computers in solving such complex tasks is therefore an important step toward accelerated materials development. Prof. Dr. Sabrina Maniscalco, CEO and co-founder of Algorithmiq, adds: "For too long, the global conversation around quantum has focused almost entirely on hardware. But hardware alone is not enough. Without major advances in algorithms and software, quantum computers risk remaining scientifically impressive without delivering meaningful industrial value. At Algorithmiq, we are building the algorithmic layer that makes quantum computers actually useful for chemistry, life sciences, new materials, and beyond."

The partners Algorithmiq and Fraunhofer ISC will meet at the leadership level in June 2026 to discuss initial joint projects and their direction

Info Box

Algorithmiq develops quantum software that makes quantum computers usable for science and industry. Algorithmiq creates the algorithmic foundation for the next generation of quantum applications in the fields of chemistry, materials science, and the life sciences. A multidisciplinary team combines world-class expertise in quantum information theory, quantum chemistry, computational life sciences, complex systems, and software development. Headquartered in Milan with offices in Helsinki, London, and Dublin, Algorithmiq operates globally and is committed to bringing quantum computing to industrial use.

Materials science is crucial for sustainable product innovation. The **Fraunhofer Institute for Silicate Research ISC**, based in Würzburg, focuses on chemical materials research and offers solutions related to sustainable materials, manufacturing, and processing. It is part of the Fraunhofer Society, one of the leading organizations for applied research, with a focus on future-oriented key technologies and the transfer of research results to industry to strengthen our economic position and benefit our society.

Fig.1 Prof. Miriam Unterlass (left) and Prof. Sabrina Maniscalco (right) bundle research power to bring quantum computing into application for materials research. © K. Wolf and Algorithmiq

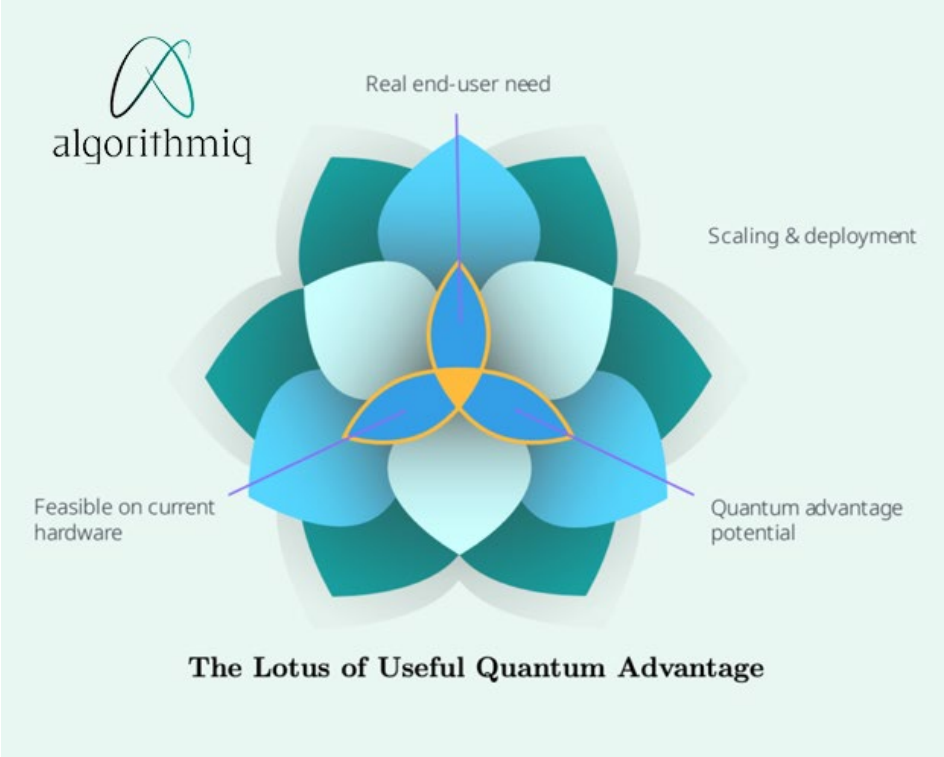

Fig.2 The lotus metaphor illustrates the path toward useful quantum advantage. The inner petals represent three conditions that must be achieved simultaneously: executability on current hardware, relevance to material space exploration, and validation against state-of-the-art classical methods under fair resource assumptions. The outer petals represent deployment, integration, and scaling. These are essential for translating advances into practice and can be systematically engineered. In a real lotus, the central structure contains the seeds that enable new flowers to grow. In the same spirit, we view this core as generative, capable of supporting multiple applications once established and are looking forward to bring this idea to materials research. © Algorithmiq

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