DR. IGOR SOKOLOV

SENIOR QUANTUM COMPUTATIONAL SCIENTIST

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Full publication list: https://scholar.google.com/citations?user=ekdwde4AAAAJ

SKILLS

- Quantum computing, AI, Software development, Quantum chemistry & physics, Scientific research, Client projects
- Python, C++, Latex, Matlab, PyTorch, JAX, Git, Qiskit, PySCF, Gaussian, PyQuante, Psi4, Openfermion, Cirq, Qutip
- Fluent in French, English, Russian, Ukrainian and B2-level German

INTODUCTION AND MOTIVATION

I am a **senior quantum computational scientist** with a strong track record in **quantum algorithms for chemistry and machine learning**. My recent work at Pasqal includes **quantum-enhanced density functional theory** and **hybrid graph neural networks**. During my PhD at IBM, I demonstrated error-resilient quantum simulations of molecular dynamics, protein folding, advanced orbital-optimised variational algorithms and transcorrelated methods for electronic structure calculations. I **lead R&D projects with industrial partners** such as Saudi Aramco and **contribute to open-source packages** such as QEX, a differentiable quantum chemistry framework in JAX. I am currently developing **quantum error correction approaches for neutral-atom quantum computers at Pasqal**, and **building a resource-estimation framework** for fault-tolerant quantum computing applications, with a particular focus on chemistry and materials science.

I must say, I always wanted to work for NVIDIA. Now, given your recent investments in quantum technologies through the NVIDIA Accelerated Quantum Research Center and the development of platforms such as CUDA-Q. These efforts are truly transformative for the future of quantum computing. With extensive experience in quantum algorithm development—including my role as a **developer of Qiskit at IBM**—and **my recent work at Pasqal leading industrial collaborations**, I am confident in my ability to make meaningful contributions to quantum science at NVIDIA including developement NVIDIA's CUDA-Q Libraries.

EDUCATION AND KEY QUALIFICATIONS

DOCTORAL DEGREE IN COMPUTATIONAL SCIENCE
IBM Research – Zürich & University of Zürich, Switzerland — 2019-2022

MASTER'S DEGREE IN PHYSICS – GRADE: 5.75/6 (CH), 9/10 (NL), A (US)
ETH Zürich, Switzerland — 2016 - 2018

BACHELOR'S DEGREE IN PHYSICS
EPF Lausanne, Switzerland — 2012 - 2016

CURRENT POSITION

PASQAL — SENIOR QUANTUM ALGORITHM DEVELOPER
Amsterdam, Netherlands — April 2022 – Now
Project(s): Quantum graph ML & Differentiable quantum chemistry
Clients: Aramco & Schrödinger
Role(s): Research leader
Technologies: Quantum neural networks
Responsibilities & Results:

- **Quantum graph ML:** Developed a scalable quantum-classical hybrid graph model with provable advantages for specific families of graphs in comparison to classical graph neural networks. Shown a two percent improvement over the state-of-the-art.
- **Quantum chemistry:** Patented the integration of quantum neural networks in density functional theory enabling computation of molecular properties and shown a ten-fold reduction in the number of training parameters in comparison to classical models.
- **Client projects:** Developed quantum-enhanced ML models for clients and their use cases.

PREVIOUS EXPERIENCE

IBM RESEARCH – ZÜRICH — PHD STUDENT
Zürich, Switzerland — December 2018 – March 2022
Project: Quantum algorithms for chemistry @ Ivano Tavernelli's lab
Technologies: Quantum algorithms
Responsibilities & Results:

- Shown how variational quantum algorithms can outperform classical projective approaches for chemistry and introduced orbital optimization that reduced the energy errors by ten-fold.
- Performed molecular dynamics simulations on a quantum computer showing resilience of the computation of molecular forces to errors in quantum hardware.

- Integrated quantum algorithms in transcorrelated methods, showing orders of magnitude reduction of errors in quantum simulations.

ETH ZÜRICH — **STUDENT ASSISTANT**
Zürich, Switzerland — July 2018 – November 2018
Project: Quantum algorithms for chemistry @ Manfred Sigrist's lab — **Technologies:** Quantum algorithms
Responsibilities & Results:
- Investigated quantum simulations for molecules presenting strong electronic correlation for future PhD studies at IBM.

IBM RESEARCH – ZÜRICH — **INTERN**
Zürich, Switzerland — May 2018 - July 2018
Project: Quantum algorithms for chemistry @ Ivano Tavernelli's lab — **Technologies:** Quantum algorithms
Responsibilities & Results:
- Finalised a publication about simulating systems exhibiting strong electronic correlation.

ETH ZÜRICH — **INTERN**
Zürich, Switzerland — July 2017 – August 2017
Project: Experimental physics @ Jérôme Faist's lab — **Technologies:** Quantum optics
Responsibilities & Results:
- Constructed a cleaner for Helium-based cooling of an ultra-strong coupling experiment.

EMPA — **VISITING SCIENTIST**
Zürich, Switzerland — June 2017 – July 2017
Project: Quantum chemistry @ Daniele Passerone's lab — **Technologies:** Computational chemistry frameworks
Responsibilities & Results:
- Performed TD-DFT simulations of graphene nano-ribbons for a study of absorption spectra.

RESEARCH ACHIEVEMENTS

Over the past 6+ years, I have developed and implemented quantum algorithms for electronic structure, density functional theory, and quantum machine learning. My PhD research introduced orbital-optimized variational methods (refs. 8-9), transcorrelated approaches (refs. 3, 5), alchemical optimization (ref. 7), quantum simulations of molecular dynamics (ref. 6) and tailoring quantum circuits to particular hardware (ref. 4) — leading to multiple high-impact publications (npj Quantum Inf., Phys. Rev. Research, Chem. Sci., J. Chem. Phys., PR A). At Pasqal, I led quantum chemistry and ML projects with industrial partners such as **Saudi Aramco** and **Schrödinger**, contributing to product-relevant algorithm development for neutral atom quantum hardware. My work on quantum-enhanced graph neural networks (ref. 2) was published at **ICML 2024**, and my hybrid quantum-classical DFT framework (ref. 1) **QEX** was released as open-source software. A patented extension of quantum neural networks to density functional theory (ref. 1) has demonstrated a novel way of expressing XC functionals in the quest for a universal XC functional. These efforts reflect my deep commitment to combining algorithmic innovation with practical applicability in quantum chemistry.

Selected publications for this position, showing significant quantum chemistry, quantum computing and AI contributions:

1. **Quantum-enhanced Neural Exchange-Correlation Functionals**
   Igor O. Sokolov, *et al.*, arXiv, 2024, `https://arxiv.org/abs/2404.14258` (**Top 3 Best papers of MoML 2024 at MIT**)
   We introduced a differentiable Kohn–Sham DFT framework using quantum neural networks (QNNs) to learn exchange–correlation functionals. Our QNN-based functionals achieve chemical accuracy on both seen and unseen molecular systems, outperforming classical ML baselines using fewer parameters. This work provides a foundation for integrating quantum models into density functional theory, enabling differentiable quantum-enhanced simulations in JAX. We open-sourced this work as a package, QEX (`https://github.com/pasqal-io/qex`). *Related **patent** was also filed in 2024.*
2. **Enhancing Graph Neural Networks with Quantum Computed Encodings**
   Slimane Thabet, Igor O. Sokolov, *et al.*, arXiv, 2023, `https://arxiv.org/abs/2310.20519` (**Published at ICML 2024**) *We introduced novel positional encodings for graph transformers inspired by quantum systems, where long-range correlations emerge naturally from qubit interactions. By mapping graph topology to quantum circuit features, we developed expressive encodings that theoretically outperform standard methods like relative random walks for certain graph families. Empirically, we showed improved performance on benchmark datasets using tractable approximations of these quantum features. This work highlights how ideas from quantum computing can enhance graph representation learning and scale to large, real-world data. In fact, **best results were achieved on chemical dataset**, ZINC.*
3. **Ab Initio Transcorrelated Method enabling accurate Quantum Chemistry on near-term Quantum Hardware**
   Igor O. Sokolov (shared first authorship), *et al.*, **JCTC**, 2024, `https://pubs.acs.org/doi/10.1021/acs.jctc.4c00070`
   We introduced a noise-resilient quantum algorithm for electronic structure based on an exact transcorrelated approach, which shifts correlation into the Hamiltonian to reduce quantum resource requirements. This method yields chemically accurate (comparable to experiment) dissociation energies, for small molecules using as few as 4–6 qubits—an order of magnitude fewer than conventional methods. By enabling shallower circuits and better convergence to the basis set limit, our approach provides a practical path toward high-accuracy quantum chemistry on near-term quantum hardware.

SIGNIFICANT SOFTWARE CONTRIBUTIONS

- **Quantum-Enhanced Density Functional Theory in JAX (QEX):** JAX-based differentiable Kohn-Sham Density Functional Theory implementation for training quantum(-enhanced) neural exchange-correlation functionals, https://github.com/pasqal-io/qex

ADDITIONAL RESEARCH ACHIEVEMENTS

4. **Hardware-Tailored Diagonalization Circuits**
   Daniel Miller, Igor O. Sokolov, *et al.*, npj Quantum Inf., 2024, https://www.nature.com/articles/s41534-024-00901-1
   We present a theoretical framework for constructing hardware-tailored (HT) quantum circuits that efficiently diagonalize sets of commuting Pauli operators with minimal gate overhead. Unlike standard approaches that rely on tensor product bases or incur high SWAP costs, our method adapts circuit construction to hardware constraints, enabling more scalable implementations. We demonstrate an algorithm for grouping Hamiltonian terms into jointly HT-diagonalizable sets and show that our method reduces the number of required measurements compared to conventional strategies. Proof-of-principle experiments on cloud-based quantum devices validate the practical efficiency of our circuits.
5. **Orders of magnitude reduction in the computational overhead for quantum many-body problems on quantum computers via an exact transcorrelated method**
   Igor O. Sokolov, *et al.*, arXiv, 2022, https://doi.org/10.1103/PhysRevResearch.5.023174
   We extend transcorrelated methods to quantum simulation by combining them with an Ansatz-based imaginary-time evolution algorithm adapted to non-Hermitian Hamiltonians. This approach enables highly compact and accurate solutions for strongly correlated systems like the Hubbard model, achieving up to four orders of magnitude improvement in accuracy while using shallower circuits. We further propose a circuit-efficient implementation of imaginary-time evolution tailored to non-Hermitian settings. Hardware experiments on IBM's quantum devices validate the method. This work opens a new path for exact transcorrelated quantum simulations of realistic ab initio systems.
6. **Microcanonical and finite-temperature ab initio molecular dynamics simulations on quantum computers**
   Igor O. Sokolov *et al.*, Physical Review Research, 2021, https://doi.org/10.1103/PhysRevResearch.3.013125
   We demonstrate how variational quantum algorithms can be used to compute atomic forces for ab initio molecular dynamics simulations, despite hardware and statistical noise. We introduce error-mitigation strategies for both energy and force evaluations and propose quantum-enhanced microcanonical and Langevin dynamics algorithms for constant-energy and constant-temperature simulations. Our results show accurate molecular trajectories for small systems, including experimental validation on IBM's ibmq-athens. This work establishes the feasibility of near-term quantum devices for simulating real-time molecular dynamics.
7. **Quantum algorithm for alchemical optimization in material design**
   Panagiotis Kl. Barkoutsos, Igor O. Sokolov *et al.*, Chemical Science, 2020, https://doi.org/10.1039/D0SC05718E
   We propose a quantum algorithm to efficiently explore chemical compound space for material and drug design by leveraging an 'alchemical' Hamiltonian that encodes all candidate atomic compositions in a quantum superposition. This method jointly optimizes atomic structure and electronic properties, enabling the selection of molecules that best match a target objective. Our approach achieves favorable scaling compared to classical methods and demonstrates promising performance in both simulations and IBM Quantum hardware. This work lays the groundwork for quantum-enhanced discovery of tailored materials using near-term devices.
8. **Quantum orbital-optimized unitary coupled cluster methods in the strongly correlated regime: Can quantum algorithms outperform their classical equivalents?**
   Igor O. Sokolov *et al.*, Journal of Chemical Physics, 2020, https://doi.org/10.1063/1.5141835
   We evaluate efficient variants of the quantum Unitary Coupled Cluster (q-UCC) Ansatz-such as singlet and pair q-UCCD, in combination with orbital optimization, to tackle strongly correlated electronic systems. These reduced Ansätze significantly lower quantum resource requirements while retaining accuracy. We demonstrate that they accurately capture challenging features like bond dissociation and distortion in molecules such as H_4, H_2O, and N_2, as well as in the 1D Fermi-Hubbard model. Our results highlight the potential of resource-efficient q-CC methods to address multi-reference problems beyond the reach of classical single-reference Coupled Cluster theory.
9. **Quantum algorithms for electronic structure calculations: particle/hole Hamiltonian and optimized wavefunction expansions**
   Panagiotis Kl. Barkoutsos, Igor O. Sokolov *et al.*, Physical Review A, 2018, https://doi.org/10.1103/PhysRevA.98.022322
   We propose a quantum algorithm for electronic structure based on transforming the second-quantized Hamiltonian into the particle–hole representation, which provides a more compact and physically motivated Ansatz for the ground-state wavefunction. By combining this formulation with exchange-type gates and variational techniques such as q-UCC, we achieve accurate energy estimations using shallow quantum circuits. We demonstrate that even a single Trotter step suffices to reproduce ground-state energies of small molecules, offering clear advantages in both expressivity and resource efficiency compared to direct mappings of classical coupled-cluster methods.

PEER RECOGNITION

Top 3 best papers in AI at MoML 2024 conference, MIT — September 2024
Nominated for top 3 best papers award and a talk

Presenter at ICML 2024 (Top AI conference) — September 2024
Poster session in classical AI conference

Lead developer for IBM Quantum Challenge 2021 - Chemistry — September 2021
Designed the chemistry challenge

Best talk award at QCxQC conference — September 2020
Won the best talk prize (https://youtu.be/FaTFYWkSMsY)

INSTITUTIONAL RESPONSIBILITIES AND OUTREACH

I have supervised MSc and PhD students at both IBM and Pasqal, contributed to hackathons, and taught elements of quantum chemistry and variational methods in summer schools. I've actively participated in international research communities, contributed to open-source development (QEX and Qiskit), and organized scientific outreach activities, journal clubs (at Pasqal), at the interface of quantum computing, chemistry, and AI.

RESEARCH STATEMENT

My research focuses on developing practical quantum algorithms for chemistry and materials simulation, with an emphasis on near-term applicability. **I am particularly interested in the intersection of quantum computing for chemistry and machine learning**, where I believe we can make the current (noisy) quantum computers useful for chemistry by integrating them with AI techniques. A central theme of my work is to identify quantum features of many-body systems that can enhance classical AI models - ultimately aiming to design hybrid algorithms that leverage quantum structure to improve prediction, optimization, and generalization in AI models for chemical and material discovery. My research agenda focuses on several interrelated directions aimed at advancing the practical impact of quantum computing in chemistry and materials science:

- **Quantum computing for electronic structure**, including orbital optimization, transcorrelated methods, and variational algorithms, with a focus on integrating these techniques with AI to improve scalability and accuracy.
- **Hybrid quantum–classical frameworks**, such as differentiable DFT implemented in GPU-accelerated platforms and connected to quantum neural networks - exemplified by our open-source library QEX (Ref. 1).
- **Quantum machine learning**, particularly the development of quantum encodings for molecular graphs and their application to molecular property prediction in drug discovery, catalysis, and materials design.

REFERENCES

1. Dr. Ivano Tavernelli (IBM Research Zurich) - ita@zurich.ibm.com
2. Dr. Ali Alavi (University of Cambridge) - asa10@cam.ac.uk
3. Dr. Martin Rahm (Chalmers University) - martin.rahm@chalmers.se

ADDITIONAL INFORMATION

I enjoy organizing sporting activities. I **play tennis competitively** and also enjoy table tennis and padel. With over **15 years of classical piano training**, I have a strong passion for music and **enjoy composing both classical and jazz pieces using software**.