# Mohammad Ghazi Vakili

Staff Scientist · QC Ware
Previously Research Associate, Matter Lab, Department of Computer Science and Chemistry, University of Toronto

Google Scholar ORCID 0000-0002-2927-4975 GitHub LinkedIn

**Google Scholar:** 941 citations · h-index 17 · i10-index 20 (as of November 3, 2026)

## SUMMARY

Researcher in AI agents and machine learning for scientific discovery and near-term quantum algorithms, with applications in drug discovery, industrial optimization and self-driving laboratories. Staff Scientist at QC Ware since April 2026; previously Research Associate at the Matter Lab, University of Toronto.

## EXPERIENCE

April 2026 – Present

**Staff Scientist** – QC Ware, Remote

Until April 2026

**Research Associate** – Matter Lab, Department of Computer Science and Chemistry, University of Toronto, Toronto, Canada

- Near-term quantum algorithms (VQE, QAOA, generative quantum eigensolvers) and quantum-inspired machine learning
- Hybrid quantum–classical generative models for drug discovery; orchestration software for self-driving laboratories

Academic year 2019/2020

**Teaching – Information Systems (M.Sc.)** – Politecnico di Torino, Turin, Italy
Lessons on web programming with Python, Flask and SQLAlchemy; recorded lectures published online.

## EDUCATION

Thesis 2021

**Ph.D., Industrial IoT and Industry 4.0** – Politecnico di Torino, Turin, Italy
Thesis: "Industry 4.0: Industrial IoT enhancement and WSN performance analysis".

**M.Sc., Mechatronic Engineering** – Politecnico di Torino, Turin, Italy

**B.Sc., Telecommunications Engineering** – Urmia University, Iran

## PUBLICATIONS (32)

### Journal articles 15

15. Ignacio Gustin, Luis Mantilla Calderón, Juan B Pérez-Sánchez, Chris Crebolder, Jérôme F Gonthier, …, **Mohammad Ghazi Vakili** (14 authors). **"El agente cuántico: automating quantum simulations."** *Reports on Progress in Physics 89(7), 077602*, 2026. doi:10.1088/1361-6633/ae8933

14. Mohsen Bagherimehrab, Luis Mantilla Calderón, Dominic W Berry, Philipp Schleich, **Mohammad Ghazi Vakili**, Abdulrahman Aldossary, Jorge A Campos Gonzalez Angulo, Christoph Gorgulla, Alán Aspuru-Guzik. **"Faster algorithmic quantum and classical simulations by corrected product formulas."** *PRX Quantum 7(3), 033018*, 2026. doi:10.1103/phk5-slkl

13. **Mohammad Ghazi Vakili**, Alessandro S Nascimento, Alán Aspuru-Guzik. **"Quantum algorithms for ligand design in drug discovery."** *Expert Opinion on Drug Discovery 21(3), 245-247*, 2026. doi:10.1080/17460441.2026.2629854

12. **Mohammad Ghazi Vakili**, Christoph Gorgulla, Jamie Snider, AkshatKumar Nigam, Dmitry Bezrukov, … (25 authors). **"Quantum-computing-enhanced algorithm unveils potential KRAS inhibitors."** *Nature Biotechnology, 1-6*, 2025. doi:10.1038/s41587-024-02526-3

11. Malcolm Sim, **Mohammad Ghazi Vakili**, Felix Strieth-Kalthoff, Han Hao, Riley J Hickman, Santiago Miret, Sergio Pablo-García, Alán Aspuru-Guzik. **"ChemOS 2.0: An orchestration architecture for chemical self-driving laboratories."** *Matter 7(9), 2959-2977*, 2024. doi:10.1016/j.matt.2024.04.022

10. Javier Alcazar, **Mohammad Ghazi Vakili**, Can B Kalayci, Alejandro Perdomo-Ortiz. **"Enhancing combinatorial optimization with classical and quantum generative models."** *Nature Communications 15(1), 2761*, 2024. doi:10.1038/s41467-024-46959-5

9. Naruki Yoshikawa, Kourosh Darvish, **Mohammad Ghazi Vakili**, Animesh Garg, Alán Aspuru-Guzik. **"Digital pipette: open hardware for liquid transfer in self-driving laboratories."** *Digital Discovery 2(6), 1745-1751*, 2023. doi:10.1039/d3dd00115f

8. Gianluca Cena, Stefano Scanzio, **Mohammad Ghazi Vakili**, Claudio Giovanni Demartini, Adriano Valenzano. **"Assessing the effectiveness of channel hopping in IEEE 802.15.4 TSCH networks."** *IEEE Open Journal of the Industrial Electronics Society 4, 214-229*, 2023. doi:10.1109/ojies.2023.3287943

7. Antonio Costantino Marceddu, Gaetano Quattrocchi, Alessandro Aimasso, Edoardo Giusto, Leonardo Baldo, **Mohammad Ghazi Vakili**, Matteo Davide Lorenzo Dalla Vedova, Bartolomeo Montrucchio, Paolo Maggiore. **"Air-to-ground transmission and near real-time visualization of FBG sensor data via cloud database."** *IEEE Sensors Journal 23(2), 1613-1622*, 2022. doi:10.1109/jsen.2022.3227463

6. Mario Collotta, Renato Ferrero, Edoardo Giusto, **Mohammad Ghazi Vakili**, Jacopo Grecuccio, Xiangjie Kong, Ilsun You. **"A fuzzy control system for energy-efficient wireless devices in the Internet of vehicles."** *International Journal of Intelligent Systems 36(4), 1595-1618*, 2021. doi:10.1002/int.22353

5. Bartolomeo Montrucchio, Edoardo Giusto, **Mohammad Ghazi Vakili**, Stefano Quer, Renato Ferrero, Claudio Fornaro. **"A densely-deployed, high sampling rate, open-source air pollution monitoring WSN."** *IEEE Transactions on Vehicular Technology 69(12), 15786-15799*, 2020. doi:10.1109/tvt.2020.3035554

4. Stefano Scanzio, **Mohammad Ghazi Vakili**, Gianluca Cena, Claudio Giovanni Demartini, Bartolomeo Montrucchio, Adriano Valenzano, Claudio Zunino. **"Wireless sensor networks and TSCH: A compromise between reliability, power consumption, and latency."** *IEEE Access 8, 167042-167058*, 2020. doi:10.1109/access.2020.3022434

3. Gianluca Cena, Claudio G Demartini, **Mohammad Ghazi Vakili**, Stefano Scanzio, Adriano Valenzano, Claudio Zunino. **"Evaluating and modeling IEEE 802.15.4 TSCH resilience against Wi-Fi interference in new-generation highly-dependable wireless sensor networks."** *Ad Hoc Networks 106, 102199*, 2020. doi:10.1016/j.adhoc.2020.102199

2. Edoardo Giusto, **Mohammad Ghazi Vakili**, Filippo Gandino, Claudio Demartini, Bartolomeo Montrucchio. **"Quantum Pliers Cutting the Blockchain."** *IT Professional 22(6), 90-96*, 2020. doi:10.1109/mitp.2020.2974690

1. Mahdieh Khalilinezhad, Ahmad Nadali, Niloufar Dehghani, **Mohammad Ghazivakili**. **"A Fuzzy Expert System for Assessing the Internet Stores Based on Web Site Attributes."** 2013. link

### Conference papers 9

9. Jiaru Bai, Abdulrahman Aldossary, Thomas Swanick, Marcel Müller, Yeonghun Kang, Zijian Zhang, Jin Won Lee, Tsz Wai Ko, Varinia Bernales, Alan Aspuru-Guzik. **"El Agente Gráfico: Structured Execution Graph for Scientific Agents."** *AI4X – Accelerate Conference 2026*, 2026. link

8. Giuseppe Barillaro, Andrea Boella, Filippo Gandino, **Mohammad Ghazi Vakili**, Edoardo Giusto, … (11 authors). **"Comparison of heuristic approaches to PCI planning for quantum computers."** *2023 IEEE International Conference on Consumer Electronics (ICCE), 1-6*, 2023. doi:10.1109/icce56470.2023.10043394

7. Renato Ferrero, **Mohammad Ghazi Vakili**, Edoardo Giusto, Mauro Guerrera, Vincenzo Randazzo. **"Ubiquitous fridge with natural language interaction."** *2019 IEEE International Conference on RFID Technology and Applications (RFID-TA), 404-409*, 2019. doi:10.1109/rfid-ta.2019.8892025

6. **Mohammad Ghazi Vakili**, Claudio Demartini, Mauro Guerrera, Bartolomeo Montrucchio. **"Open source fog architecture for industrial IoT automation based on industrial protocols."** *2019 IEEE 43rd Annual Computer Software and Applications Conference (COMPSAC) 1, 570-578*, 2019. doi:10.1109/compsac.2019.00088

5. **Mohammad Ghazivakili**, Claudio Demartini, Claudio Zunino. **"Industrial data-collector by enabling OPC-UA standard for Industry 4.0."** *2018 14th IEEE International Workshop on Factory Communication Systems (WFCS), 1-8*, 2018. link

4. Masoud Hemmatpour, **Mohammad Ghazivakili**, Bartolomeo Montrucchio, Maurizio Rebaudengo. **"DIIG: a distributed industrial IoT gateway."** *2017 IEEE 41st Annual Computer Software and Applications Conference (COMPSAC) 1, 755-759*, 2017. link
3. Mahdieh Khalilinezhad, Ahmad Nadali, **Mohammad Ghazivakili**. **"Evaluating online shopping stores based on web site attributes using fuzzy expert system."** *Proceedings of the International Conference on Advances in Computer Science and Applications, 70-76*, 2012. link
2. Ahmad Nadali, Pouria Goldasteh, **Mohammad Ghazivakili**, Sami Ahmari. **"Evaluating success of innovation ideas in social computing technologies using fuzzy expert system."** *2012 Third FTRA International Conference on Mobile, Ubiquitous, and Intelligent Computing, 78-83*, 2012. link
1. Pouria Goldasteh, Ahmad Nadali, **Mohammad Ghazivakili**, Sami Ahmari. **"A Fuzzy Expert System for Evaluating Value Innovation in Social Computing Platforms Based on Blue Ocean Strategy (Case Study: WBB Platform)."** *Proceedings on the International Conference on Internet Computing (ICOMP), 1*, 2012. link

### Preprints 6

6. Juan B Pérez-Sánchez, Yunheng Zou, Jorge A Campos-Gonzalez-Angulo, Marcel Müller, Ignacio Gustin, ..., **Mohammad Ghazi Vakili** (15 authors). **"El Agente Quntur: A research collaborator agent for quantum chemistry."** *arXiv preprint arXiv:2602.04850*, 2026. doi:10.1016/j.chempr.2026.103259
5. Changhyeok Choi, Yunheng Zou, Marcel Müller, Han Hao, Yeonghun Kang, ..., **Mohammad Ghazi Vakili** (13 authors). **"El agente estructural: An artificially intelligent molecular editor."** *arXiv preprint arXiv:2602.04849*, 2026. doi:10.48550/arxiv.2602.04849
4. Luca Thiede, Abdulrahman Aldossary, Andreas Burger, Jorge Arturo Campos-Gonzalez-Angulo, Ning Wang, ..., **Mohammad Ghazi Vakili** (12 authors). **"Coupled Cluster con MōLe: Molecular Orbital Learning for Neural Wavefunctions."** *arXiv preprint arXiv:2602.20232*, 2026. doi:10.48550/arxiv.2602.20232
3. Kimberlee Keithley, Shunsuke Yamamoto, Ryota Kenmoku, Ikko Hamamura, Kouhei Nakaji, ..., **Mohammad Ghazi Vakili** (19 authors). **"Auger Spectroscopy via Generative Quantum Eigensolver: A Quantum Approach to Molecular Excitations."** *arXiv preprint arXiv:2603.12859*, 2026. doi:10.48550/arxiv.2603.12859
2. Kouhei Nakaji, Lasse Bjørn Kristensen, Ryota Kemmoku, Jorge A Campos-Gonzalez-Angulo, **Mohammad Ghazi Vakili**, ... (17 authors). **"The generative quantum eigensolver (GQE) and its application for ground state search."** *arXiv preprint arXiv:2401.09253*, 2024. doi:10.48550/arxiv.2401.09253
1. **Mohammad Ghazi Vakili**, Christoph Gorgulla, AkshatKumar Nigam, Dmitry Bezrukov, Daniel Varoli, ... (22 authors). **"Quantum Computing-Enhanced Algorithm Unveils Novel Inhibitors for KRAS."** *arXiv e-prints, arXiv: 2402.08210*, 2024. doi:10.48550/arxiv.2402.08210

### Thesis 1

1. **Mohammad Ghazivakili**. **"Industry 4.0: Industrial IoT enhancement and WSN performance analysis."** *Ph.D. thesis, Politecnico di Torino*, 2021. link

### Datasets 1

1. Stefano Scanzio, **Mohammad Ghazivakili**, Gianluca Cena, Claudio Giovanni Demartini, Bartolomeo Montrucchio, Adriano Valenzano, Claudio Zunino. **"From Real Data of Wireless Sensor Networks based on TSCH, to a Prediction of Reliability, Power Consumption, and Latency (dataset)."** *Dataset, Politecnico di Torino*, 2020. doi:10.21227/fg62-bp39

---

Generated from Google Scholar and the site's profile data on November 3, 2026. The latest version is always on the website.