

The Electron Density: A Fidelity Witness for Quantum Computation

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Description

Electron densities calculated using physical (superconducting qubits) and simulated quantum computers for the hydrogen molecule (H₂), lithium hydride (LiH), di-lithium (Li₂), and hydrogen cyanide (HCN). Additionally, the reduced one-particle density matrix (1-RDM) and results of topological analysis for the mentioned molecules. Calculations on physical quantum hardware were performed on Särinmer, a quantum processor with three superconducting qubits. Simulations of quantum computers were performed with Qiskit.

Data contains personal data

No

Language

[English](#)

Data format / data structure

[Numeric](#)

Data collection 1

- Mode of collection: Physical measurements and tests
- Description of the mode of collection: Calculations performed on quantum computers

- Data collector: Chalmers University of Technology

Data collection 2

- Mode of collection: Simulation
- Description of the mode of collection: Simulations of noise and noise-free quantum computers
- Data collector: Chalmers University of Technology

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Funding 1

- Funding agency: European Commission
- Funding agency's reference number: HORIZON-CL4-2022-QUANTUM-01-SGA
- Project name on the application: OpenSuperQPlus100

Funding 2

- Funding agency: Swedish Research Council
- Funding agency's reference number: 2022-06725
- Project name on the application: NAISS

Funding 3

- Funding agency: Wallenberg Center for Quantum Technology (WACQT)

Funding 4

- Funding agency: Swedish Research Council
- Funding agency's reference number: 2018-0597

Funding 5

- Funding agency: European Commission
- Funding agency's reference number: 101062864
- Project name on the application: Marie Skłodowska-Curie grant

Funding 6

- Funding agency: European Commission
- Funding agency's reference number: H2020-FETFLAG-2018-03
- Project name on the application: OpenSuperQ

Research area

[Theoretical chemistry](#) (Standard för svensk indelning av forskningsämnen 2011)

[Other physics topics](#) (Standard för svensk indelning av forskningsämnen 2011)

Keywords

[Computational chemistry](#), [Quantum computers](#), [Electronic structure](#)

Publications

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Accessibility level

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Versions

Version 1. 2024-01-11

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[Accelerating Variational Quantum Eigensolver Convergence using Parameter Transfer](#)

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