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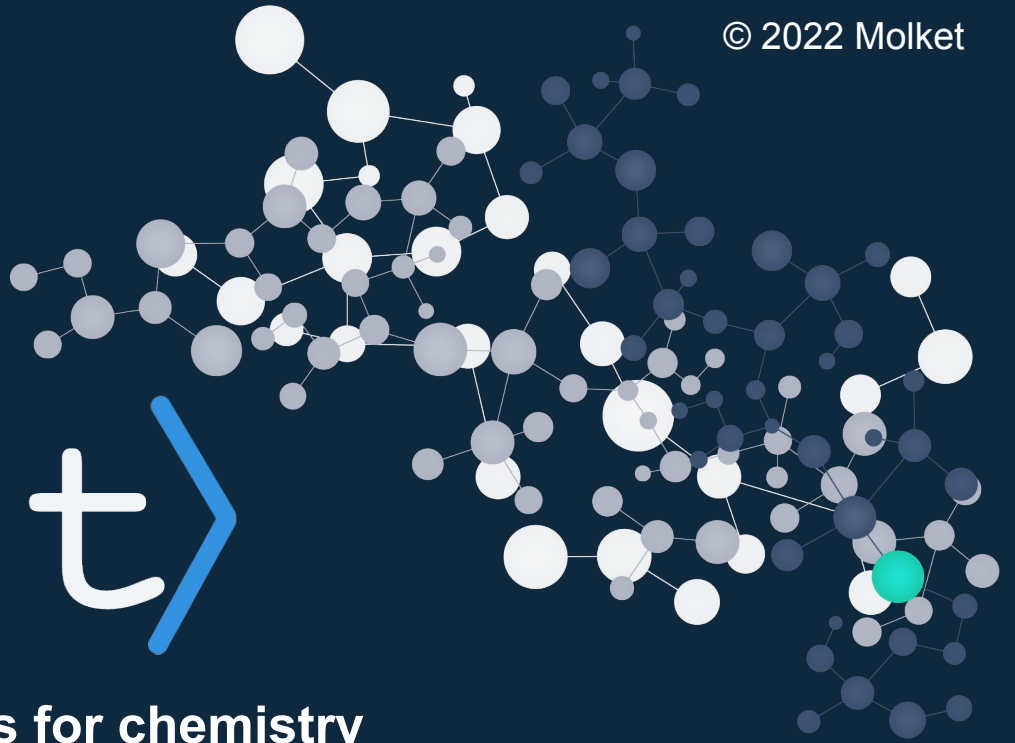

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Algorithms & Software services for chemistry using classical/quantum computers

Fast and accurate molecular simulations

Taha Selim
Alain Chancé

We deliver cost/accurate efficient molecular simulations on classical/quantum computers

Computational/simulation Software services:

1 - Mathematical modelling
2 - algorithm & code development
3 - Commercial packages
4 - Whitepapers & scientific papers
4 - consultancy
5 - training

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We use our expertise in *molecular simulations*

Taha Selim

Theoretical & Computational Chemist
Algorithm and Software developer
Founder, MolKet (NL)
LinkedIn: tiselim

Alain Chancé

Quantum Software/Research Engineer
IBM Certified Associate Developer
Founder & CEO of Quantalain SASU (FR)
LinkedIn: alainchance

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Taha Selim

- Theoretical/Computational Quantum Chemist/physicist and algorithm developer and engineer
- Published with his promoters new computational methods, algorithms, and codes for quantum molecular dynamics (references at the end).
- Founder of *MolKet*, the Netherlands, A spin off Radboud University Nijmegen.
-
- Founder & Developer at *codemath.ai*: an online free platform to teach computational physics
- A graduating Ph.D. in the theoretical and computational chemistry/physics, Institute of Molecules & Materials (IMM), Radboud University Nijmegen (RU), the Netherlands
- Software application engineer & teacher at the physics department (RU-NL).

LinkedIn: https://www.linkedin.com/in/tiselim/

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Alain Chancé

- Founder & CEO of Quantalain SASU, Paris, France, which provides business management consulting services to deep tech startups.
- Co-author of the book titled: "*Quantum Chemistry and Computing for the Curious: Illustrated with Python and Qiskit® code*".
- Successfully completed a number of Qiskit hackathons since 2018. Qiskit Advocate.
- IBM Certified Associate Developer - Quantum Computation using Qiskit v0.2X.
- Diploma ingénieur civil des Mines from École des Mines de Saint-Étienne (1981).

LinkedIn: https://www.linkedin.com/in/alainchance/

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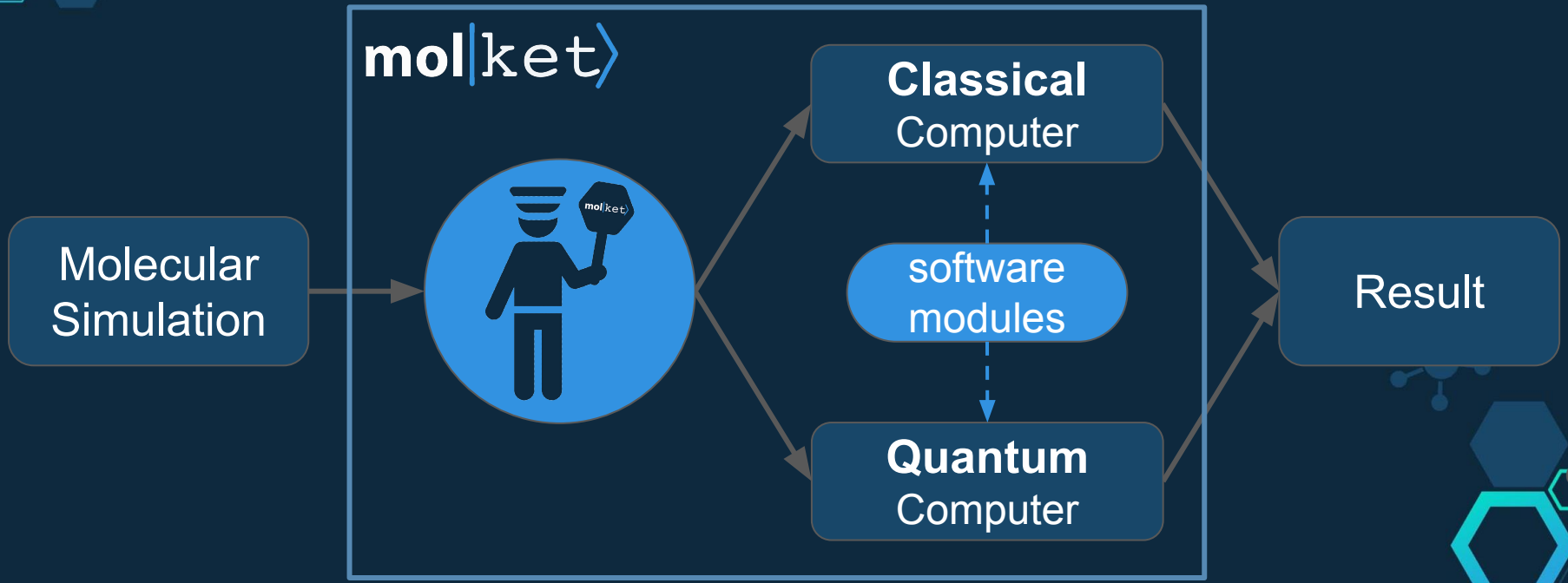
Services by hybrid classical/quantum computing



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Software Services

Consulting

1. Scoping an accurate quantum chemistry molecular simulation project.
2. Launching a request for proposal for computational platforms and selecting a few.

Designing, developing and benchmarking an accurate molecular simulation

1. Performing a first approximate simulation with commercial & open source packages.
2. Designing a mathematical model of the Hamiltonian of the molecule.
3. Implementing the mathematical model and optimizing the code.
4. Benchmarking the simulation on a selection of computing platforms.
5. Looping back to step 2 until the target accuracy and cost of computation is reached.

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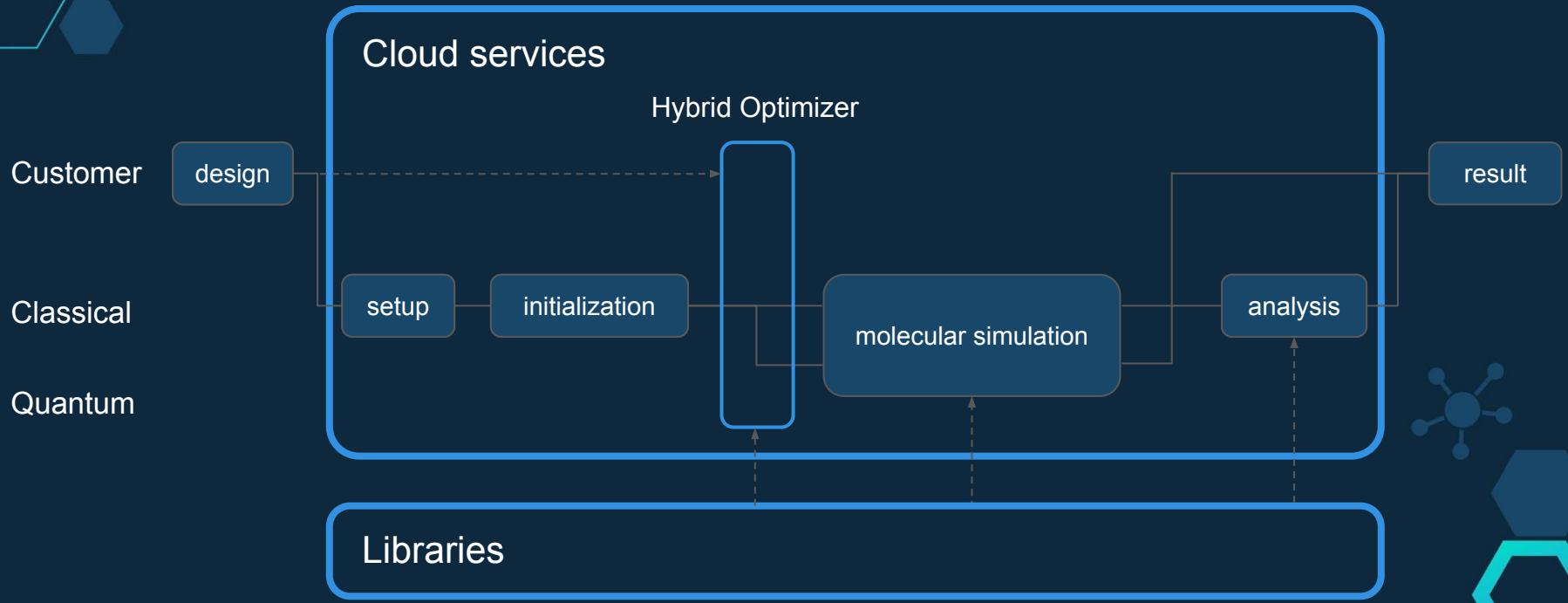
Product layout



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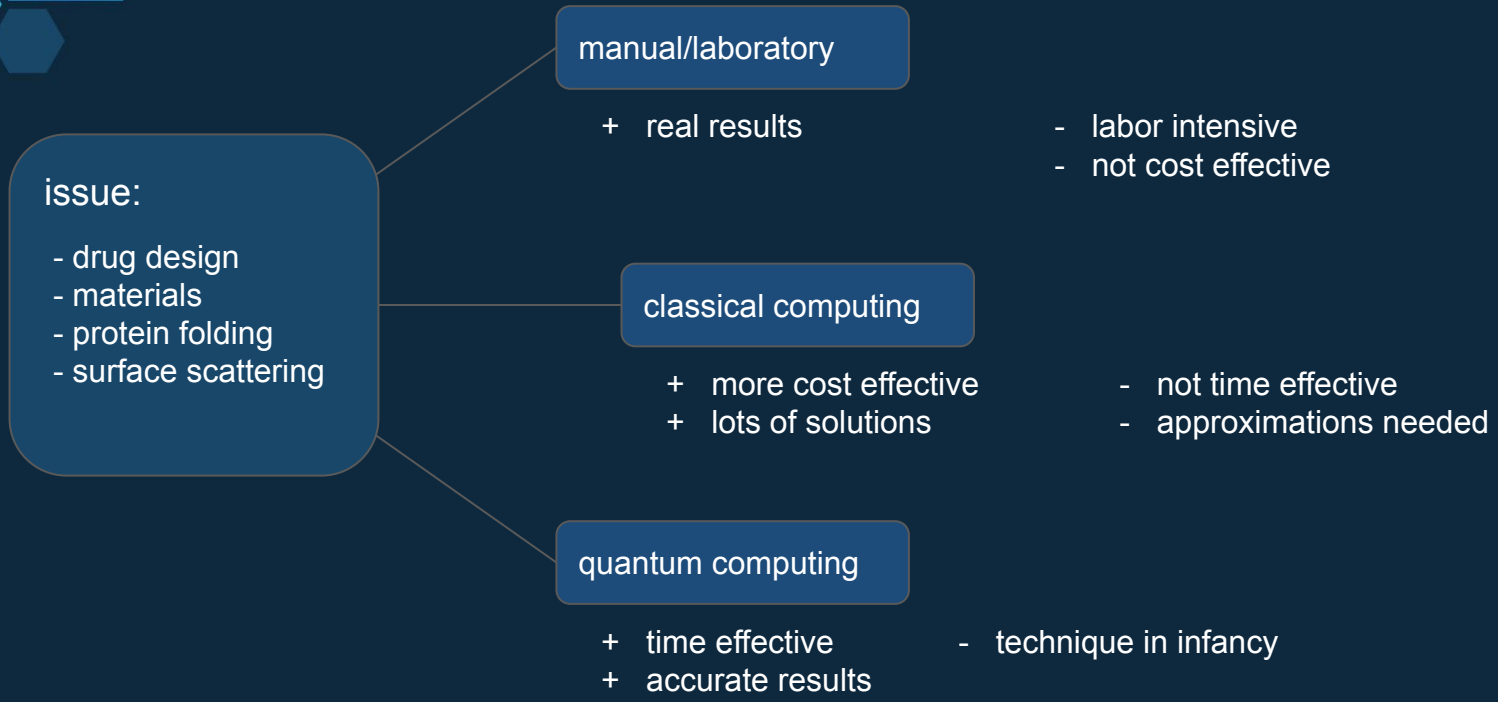
Market potential



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PhD Publications by Taha Selim

- ”Multi-channel distorted-wave Born approximation for rovibrational transition rates in molecular collisions”, Taha Selim, Arthur Christianen, Ad van der Avoird, and Gerrit C. Groenenboom, J. Chem. Phys. 155, 034105 (2021): https://doi.org/10.1063/5.0058576.

- ”Efficient computational methods for rovibrational transition rates in molecular collisions”, Taha Selim, Ad van der Avoird, and Gerrit C. Groenenboom, J. Chem. Phys.(in press) (2022): Accepted: 11 July 2022: https://doi.org/10.1063/5.0102224 arXiv: https://doi.org/10.48550/arXiv.2206.04470.

- ”Collision rates of the bend-overtone rovibrational transitions in CO_2 induced by collisions with He (Fermi Resonance)”, Taha Selim, Ad van der Avoird, and Gerrit C. Groenenboom, *in preparation*.

- ”Collision rates of the bend-mode rovibrational transitions in CO_2 induced by collisions with He”, Taha Selim, Ad van der Avoird, and Gerrit C. Groenenboom, t*o be submitted to the Journal of Chemical Physics (JCP)*.

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