

# mol ket

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 & consulting services:

- 1 Mathematical modelling
- 2 Algorithm & code development
- 3 Commercial packages
- 4 Whitepapers & scientific papers
- 4 Consultancy
- 5 Training



# We use our expertise in molecular simulations



Taha Selim

Theoretical & Computational Chemist Algorithm and Software developer CEO & Founder of MolKet (NL)

LinkedIn: tiselim



**Alain Chancé** 

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



#### 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: <a href="https://www.linkedin.com/in/tiselim/">https://www.linkedin.com/in/tiselim/</a>



#### **Alain Chancé**

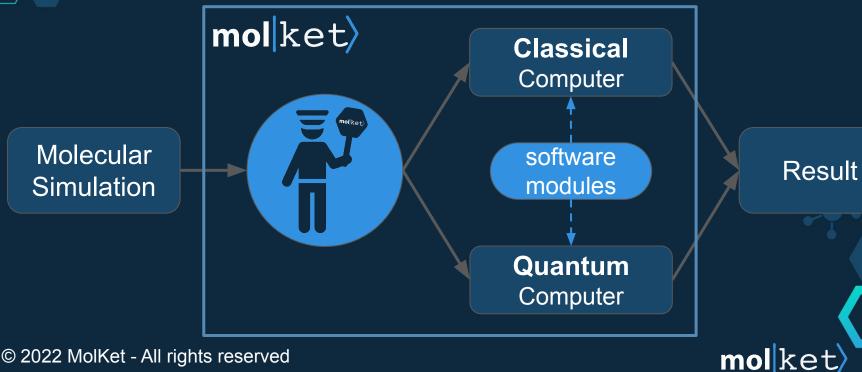
- Founder & CEO of Quantalain SASU, Paris, France, which provides business management consulting services to deep tech startups.
- Co-author of the book titled: "Quantum Chemistry and Computing for the Curious: Illustrated with Python and Qiskit® code".
- Successfully completed a number of Qiskit hackathons 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/





#### Services by hybrid classical/quantum computing





#### Consulting and Software Services

#### Consulting

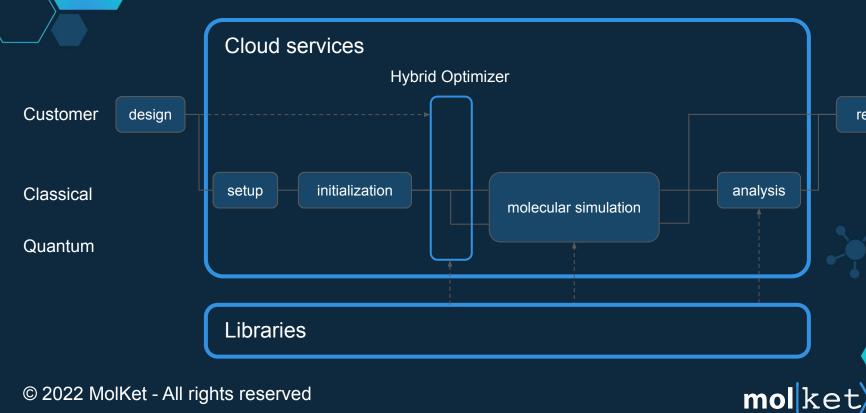
- 1. Scoping an accurate quantum chemistry molecular simulation project.
- 2. Launching a request for proposal for computational platforms and selecting a few.

#### 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



## Product layout



result

#### Market potential

#### issue:

- drug design
- materials
- protein folding
- surface scattering

#### manual/laboratory

+ real results

- labor intensive
- not cost effective

#### classical computing

- + more cost effective
- + lots of solutions

- not time effective
- approximations needed

#### quantum computing

- + time effective
- accurate results
- technique in infancy



#### PhD Publications by Taha Selim

- "Multi-channel distorted-wave Born approximation for rovibrational transition rates in molecular collisions", <u>Taha Selim</u>, Arthur Christianen, Ad van der Avoird, and Gerrit C. Groenenboom, J. Chem. Phys. 155, 034105 (2021): <a href="https://doi.org/10.1063/5.0058576">https://doi.org/10.1063/5.0058576</a>.
- "Efficient computational methods for rovibrational transition rates in molecular collisions", <u>Taha Selim</u>, Ad van der Avoird, and Gerrit C. Groenenboom, J. Chem. Phys.(in press) (2022): Accepted: 11 July 2022: <a href="https://doi.org/10.1063/5.0102224">https://doi.org/10.1063/5.0102224</a> arXiv: <a href="https://doi.org/10.48550/arXiv.2206.04470">https://doi.org/10.48550/arXiv.2206.04470</a>.
- "Collision rates of the bend-overtone rovibrational transitions in CO<sub>2</sub> induced by collisions with He (Fermi Resonance)", <u>Taha Selim</u>, Ad van der Avoird, and Gerrit C. Groenenboom, *in preparation*.
- "Collision rates of the bend-mode rovibrational transitions in CO<sub>2</sub> induced by collisions with He",
   <u>Taha Selim</u>, Ad van der Avoird, and Gerrit C. Groenenboom, to be submitted to the Journal of Chemical Physics (JCP).

