QPFAS: Quantum Chemistry Platform for Elimination of PFAS Molecules

ICHEC Irish Centre for High-end Computing · accenture · IONQ

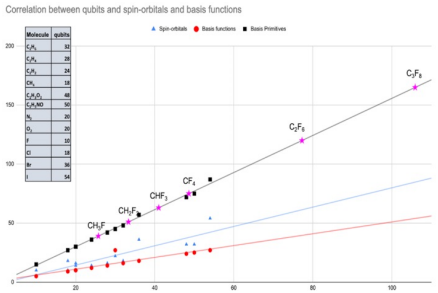
Quantum Computing Approach to Computational Chemistry

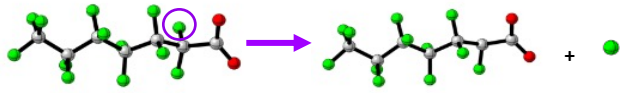
CHALLENGE

- PFAS[1] are human-made compounds used for waterproof clothing, food packaging, etc. **PFAS don't biodegrade, a.k.a. "the forever chemical."** They build up in humans and the environment; and cause a host of **detrimental health effects including cancer.**
- Finding mechanisms to destroy/remove PFAS from the ecosystem is a **global environmental challenge.**
- Using computational methods for **exact simulation of PFAS chemistry** (at the level of molecular quantum mechanics) to find pathways for their destruction is **beyond the limits of current supercomputers**.
- Can we use **quantum computing** to study the electronic structure of PFAS molecules and the molecular dynamics of PFAS reactions?

APPROACH

- Researchers from **ICHEC, Accenture, and IonQ** collaborated to build a hybrid **quantum computing solution** for running large number of computational chemistry experiments on both HPC and a quantum computer.
- After chemistry studies we identified the target problem to be the calculation of **bond disassociation curve for carbon-fluorine bond** in small PFAS.

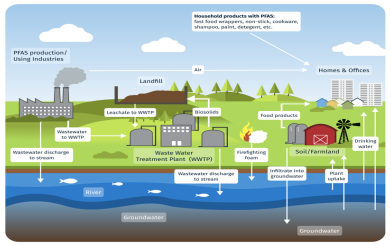


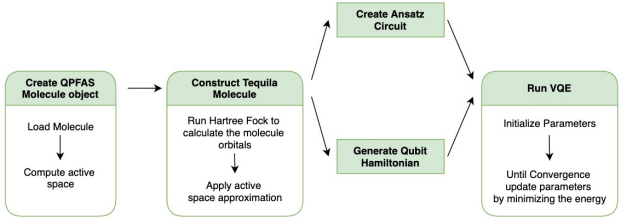


$C_6F_{13}\text{-}COO^- \longrightarrow C_6F_{12}\text{-}COO^- + F$

Defluorination : Destruction of PFAS by breaking a C-F bond

Assessing the viability of molecules for analysis with respect to number of qubits needed.

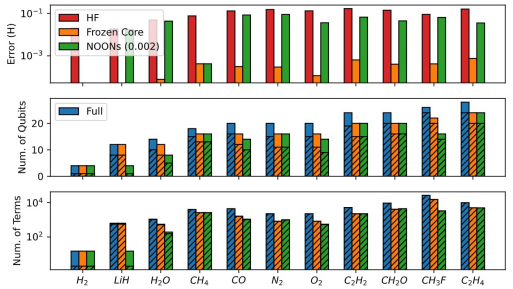




The workflow of the VQE orchestration platform

OUTCOMES

- We built a **novel scalable quantum chemistry platform** that allows running end-to-end chemistry experiments on HPC and quantum computers.
- It solves the electronic structure problem using VQE algorithm with many custom components to enable large simulations.
- Researchers can specify a wide set of parameters for many experiments, then the platform **creates parallel jobs and orchestrates their execution** on an HPC or quantum hardware and collects all the results in a database.
- We **calculated bond breaking energies for several molecules** (including small PFAS) on an HPC (Ireland's national HPC Kay) and IonQ's quantum hardware,
- The results are crucial to understanding the state-of-the-art with quantum chemistry and planning for the future of this technology.
- The solution **can be applied to a wide range of other use cases** such as discovery of drugs, sustainable fertilizers, and carbon capture methods.



Comparison of the needed resources (qubits) and obtained accuracy for various molecules using different methods, based on our extensive simulations.

1) Per- and Polyfluoroalkyl Substance ~4.700 different compounds