

Accelerating the molecular search behind better fuels and materials.

bp and ORCA built a hybrid quantum-classical model that finds low-energy molecular structures more precisely than a classical model — the shapes that determine how a biofuel burns or how a material performs.

CONFORMERS

50%

more precise energy targeting vs a classical generative model, half the standard deviation across all tested conditioning energies

8%

closer angle distribution to ground truth vs classical models, more accurate molecular shape generation

1. Hitting a computational wall

A molecular conformation is the 3D shape a molecule adopts, and that shape governs its physical, chemical, and biological properties. Generating realistic low-energy conformers, the most stable and most useful ones, is central to fuels and chemical research and development.

This search to achieve the optimum shape-space conformation is becoming computationally unfeasible to process on classical systems alone, and is a commercial bottleneck for the industry.

2. Benchmark results

Working with bp, ORCA benchmarked the hybrid GAN against an identical, purely classical model, producing conformers twice as concentrated around the target energy with a dihedral angle distribution 8% closer to ground truth. Conformers were generated close to a specified low energy in a similar time to traditional approaches, with accuracy maintained as molecule size scales.

3. The value that ORCA delivers

bp and ORCA built a hybrid quantum-classical generative adversarial network (GAN) that uses a quantum prior to seed a classical generative model conditioned on a target energy.

This approach aims to generate low-energy conformations of small and medium-sized hydrocarbon molecules, offering a solution to the computational hurdles faced in molecular exploration.

USE-CASE IMPLEMENTATION

Hybrid solution

PT-2 photonic quantum accelerator (48 qumodes)

Classical HPC with NVIDIA GPUs

ORCA SDK with Python and PyTorch compatibility

AI approach

Quantum-accelerated GAN for conformer generation