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Some steps towards enabling practical quantum computing of biomolecules

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Abstract

Quantum computers hold the promise of simulating biomolecules that are currently beyond the reach of even the most advanced quantum chemistry theories. In the last five years, there's been a notable increase in studies using quantum computers for these calculations. While the field has seen considerable advancements, we're still some way from using quantum computers for practical calculations. In this talk, I'll shed light on our latest efforts to close this gap. It's important to note that quantum computers have specific strengths, and to unlock their full potential for quantum chemistry, better integration with classical computers is essential. We're working on this integration and have pioneered techniques such as quantum-selected configuration interaction (QSCI) and computational basis sampling. I'll talk about hybrid algorithms we've developed that combine the strengths of quantum and classical computing.